

# NUCLEAR CRITICALITY SAFTEY PROGRAM (NCSP)

**FY2019 Q1 QUARTERLY REPORTS** 

NCSP Element and Subtask: LANL AM1, AM2, AM4, AM5, AM6

Task Title: see last page

M&O Contractor Name: LANL

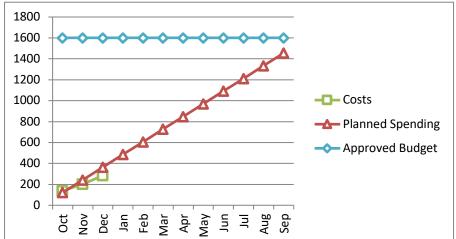
Point of Contact Name: Bob Margevicius / Bob Little Point of Contact Phone: 505-665-8965 / 505-665-3487

# MAJOR ACCOMPLISHMENTS

Reference: B&R DP0909010

Date of Report: January 24, 2019





- 1. Carryover into FY 2019 = \$0
- 2. Approved FY 2019 Budget = \$1,601,000 (includes carryover)
- 3. Actual spending for  $1^{st}$  Quarter FY 2019 = \$283,516
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$
- 6. Actual spending for  $4^{rd}$  Quarter FY 2019 = \$
- 7. Projected carryover into FY 2020 = \$146,000

### MCNP R&D Work, continued to investigate & develop (AM1)

- region-dependent sensitivity-uncertainty data for NCS validation
- fission matrix methods to diagnose & accelerate MC source convergence
- diagnostic tests for undersampling & clustering
- ENDF/B-VIII.0 data & effects on results for MCNP validation suites
- machine learning studies to understand the bias in criticality calculations and alternative ways to cluster similar benchmarks together
- impact of correlated fission multiplicity models in criticality calculations
- studies into the validation for chlorine
- impact of excluding benchmark outliers on the Whisper selection of similar benchmarks & on the Whisper baseline-USLs.
- new & improved methods for static-alpha eigenvalue calculations

### • MCNP Support & Maintenance (AM1)

 Code modernization effort - Efforts are in progress to improve SQA, implement some MCNP-2020 features, & upgrade portions of MCNP6. Includes more formal planning, design proposals, improved code review, SOA tools, and more. (Most of funding is non-NCSP.)

### • Monte Carlo Education (AM1)

- Thesis advisor for UNM graduate student working in area of criticality calculations
- Completed UNM Monte Carlo class for undergraduate & graduate students,
   20 students
- **Milestone completed:** Collected reports on summer intern work accomplished in 2018, see list of reports & publications below.

### • Comparison of Sensitivity-Uncertainty-based USL Methods (AM4)

 Comparison of results from LANL & ORNL is in progress. Awaiting results from IRSN.

### • Comparison of ICSBEP Benchmark Results (AM5)

Preliminary results were obtained from LANL, LLNL, ORNL, SNL, IRSN. Detailed comparison of results will occur in 2019.

### Technical Data for the Pitzer Formulation of Solution Compositions (AM6)

 Participated in teleconference with ORNL and LLNL, transmitted density data for uranium sulfate, literature search progressing for additional density data.

### NJOY Development and Support (AM2)

- Delivered NJOY development and maintenance plan.
- Continued to support NJOY users via emails sent to <u>njoy@lanl.gov</u> as well as issues submitted on GitHub.
- On track to deliver modernized Doppler broadening capabilities for NJOY21 in Q2
- Starting work on modernization of ACER.

### • Reports & Publications

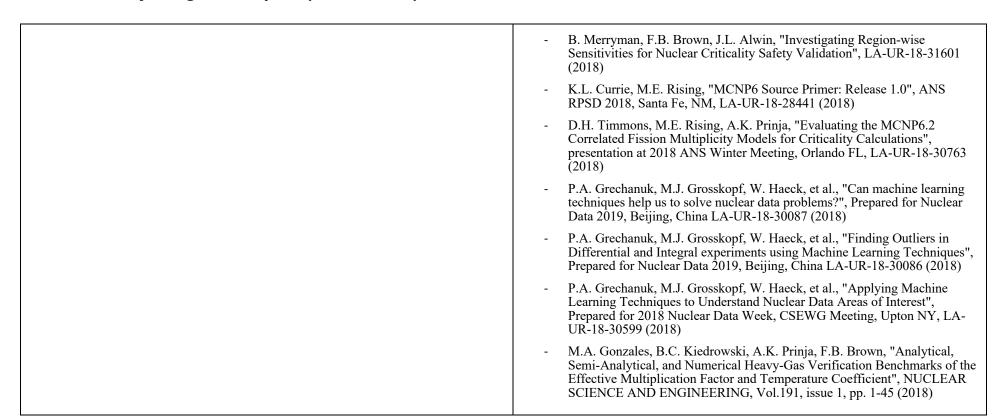
- J.L. Alwin, F.B. Brown, M.E. Rising, "Excluding Benchmark Statistical Outliers in Nuclear Criticality Safety Validation: A Comparison Study of Upper Subcritical Limits for Plutonium Systems using Whisper-1.1", LA-UR-18-27731 (2018)
- J.L. Alwin, F.B. Brown, "Excluding Benchmark Statistical Outliers in Nuclear Criticality Safety Validation: A Comparison Study of Upper Subcritical Limits for Highly Enriched Uranium Systems", submitted to ANS Annual Meeting 2019, Minneapolis MN, LA-UR-19-20048; 2019-01-08
- J.A. Alwin, F.B. Brown, "Excluding Statistical Outliers in Nuclear Criticality Safety", submitted to ANS Annual Meeting 2019, Minneapolis MN, LA-UR-19-20084 (2019)

- M.E. Rising, "MCNP6 Code Developments and CGMF/FREYA Integration and Validation", LA-UR-18-26533 (2018)
- F.B. Brown, M.E. Rising, J.L. Alwin, "Verification of MCNP6.2 for Nuclear Criticality Safety Applications", presentation at 2018 ANS Winter Meeting, Orlando FL, LA-UR-18-30510 (2018)
- C.J. Solomon, M.E. Rising, "(U) Modernization of the Monte Carlo N-Particle Transport Code", LA-CP-18-00110 (2018)
- S.R. Bolding, C.J. Josey, M.E. Rising, C.J. Solomon, J.S. Bull, "Release Testing for MCNP 6.2.1", LA-UR-18-30577 (2018)
- J.L. Alwin, "MCNP6 Unstructured Mesh (UM) for Criticality Accident Alarm System (CAAS) Analysis", presentation at ANS RPSD 2018, Santa Fe NM, LA-UR-18-28059 (2018)
- J.L. Alwin, J.B. Spencer, "Criticality Accident Alarm System (CAAS) CSG-UM Hybrid Example", presentation at ANS RPSD 2018, Santa Fe NM, LA-UR-18-28060 (2018)
- Jeremy Lloyd Conlin, "Development and Maintenance of NJOY (2018 Revision), December 18, 2018

### Reports on Post-Doc Work:

- C.J. Josey, F.B. Brown, "Fitting Nuclear Data with Chebyshev Polynomials", presentation at 2018 ANS Winter Meeting, Orlando FL, LA-UR-18-30509 (2018)
- C.J. Josey, F.B. Brown, "Bias in Monte Carlo Alpha-Eigenvalue Calculations", presentation at 2018 ANS Winter Meeting, Orlando FL, LA-UR-18-30508 (2018)
- C.J. Josey, F.B. Brown, "Computing Alpha Eigenvalues Using the Fission Matrix", submitted to ANS Mathematics & Computations 2019, Portland OR, LA-UR-18-31280 (2018)
- C.J. Josey, F.B. Brown, "Stabilizing the K-Alpha Iteration Algorithm in Very Subcritical Regimes", submitted to ANS Mathematics & Computations 2019, Portland OR, LA-UR-18-31279 (2018)
- T.P. Burke, F.B. Brown, "Development of a Library for Computing Monte Carlo Tallies on Heterogeneous Systems", presentation at 2018 ANS Winter Meeting, Orlando FL, LA-UR-18-30498 (2018)

### • Reports & Publications on Student Work:



### **LANL AM Milestones:**

STATUS (copy color code and paste below in 'STATUS' field)

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Support MCNP6 users (AM1)		
	Support NJOY users (AM2)		
	Provide status reports on LANL participation in US and International analytical methods collaborations (AM1, AM2, AM4, AM5, and AM6)		
	Provide reports on summer intern work accomplished (AM1)		
Q2	Support MCNP6 users (AM1)		
	Support NJOY users (AM2)		
	Provide status reports on LANL participation in US and International analytical methods collaborations (AM1, AM2, AM4, AM5, and AM6)		
	Issue an MCNP V&V report, including ENDF/B-VIII.0 (AM1)		
	Provide MCNP6 Criticality training course (AM1)		
	Provide status of R&D and modernization efforts at the NCSP Technical Program Review (AM1)		

	T I A D I I I I I I I I I I I I I I I I I	
	Implement the Doppler broadening capabilities into the NJOY21	
	framework (AM2)	
Q3	Support MCNP6 users (AM1)	
\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	Support Merti o users (Mini)	
	Support NJOY users (AM2)	
	D 11	
	Provide status reports on LANL participation in US and	
	International analytical methods collaborations (AM1, AM2,	
	AM4, AM5, and AM6)	
	Release initial version of MCNP6 with automatic convergence	
	testing & under-sampling diagnostics to several NCSP early-	
	adopters for testing, issue report (AM1)	
Q4	Support MCNP6 users (AM1)	
	Cymraet NIOV ygaeg (AM2)	
	Support NJOY users (AM2)	
	Provide status reports on LANL participation in US and	
	International analytical methods collaborations (AM1, AM2,	
	AM4, AM5, and AM6)	
	Implement ACER fast neutron capabilities into the NJOY21	
	framework (AM2)	
	` '	
	Issue report on the Sensitivity-Uncertainty Comparison Study	
	(AM4)	
	Issue report on the ICSBEP Benchmark Comparison Study	
	1 1	
	(AM5)	
	Document and release beta versions of ENDF/B-VIII.1	
	evaluations in ACE format on LANL website (AM1)	

### Task Title:

AM1 MCNP Maintenance and Support, Uncertainty Analysis Development, and Modernization

AM2 NJOY Development and Maintenance, Uncertainty Analysis Development, and Modernization

AM4 Sensitivity/Uncertainty Comparison Study with a Focus on Upper Subcritical Limits

AM5 Proposed Benchmark Intercomparison Study

AM6 Technical Data for the Pitzer Formulation of Solution Compositions to Include Uranium/Plutonium Solutions with Selected Admixed Absorbers

# Development and Maintenance of NJOY

2018 Revision

Jeremy Lloyd Conlin

Los Alamos National Laboratory

December 18, 2018

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### 1 Introduction

NJOY is the leading nuclear data processing code, which is developed at Los Alamos National Laboratory. NJOY21 is the current production version. It replaces the legacy, Fortran-based, NJOY2016 which is a direct descendent of the original version released in 1977.

NJOY21 is the next-generation version of NJOY that is being completely modernized. It has been released with an Open Source license and has *no export control restrictions*. More information about NJOY21 can be found in Section 2.

This report serves to document the development and maintenance plan for NJOY—including legacy NJOY and NJOY21. This document is constantly being updated as the development of NJOY proceeds. The source of this document can be found in a git repository at LANL.

### 2 NJOY21—NJOY for the 21st Century

NJOY21 is the next-generation processing code produced at Los Alamos National Laboratory. It is intended as a replacement for the Legacy version of NJOY (i.e., NJOY2016) and will eventually have the same capabilities as Legacy NJOY.<sup>1</sup>

### 2.1 Vision, Mission, Goals

To facilitate the development of NJOY21 a Vision and Mission has been created as well as specific Goals we want to accomplish. These can be found on our webpage, Vision, Mission, Goals, and are repeated here. The Vision is ambitious and gives a long-term goal towards which we are working. The Mission provides a means whereby we can accomplish the Vision. The Goals are specific things we must achieve in order to make progress towards accomplish the Mission and Vision.

### Vision

NJOY21 will be the gold standard of nuclear data processing codes by providing a trusted and verified processing code that is fast, flexible, easy to use and customize, and capable of handling both modern and established nuclear data formats.

### Mission

The mission of NJOY21 is to build on the experience of previous versions of NJOY while providing a verified and validated tool to process evaluated nuclear data files that is fast, easy, and convenient.

### Goals

- I. Maintain NJOY's image of a trusted and stable processing code
  - 1. Verified and validated—Every function and feature is automatically, frequently, and regularly tested.
  - 2. Every feature of NJOY will be documented.
  - 3. Remain backwards compatible with NJOY2016.
  - 4. Provide tools for verification of formats and validation of data.

### II. Easier

- Easier to build NJOY
  - Simple build system for all supported platforms
  - Fully automated build system—about 5 commands required to build, regardless of platform
- Easier to verify and validate NJOY

<sup>&</sup>lt;sup>1</sup>There will be some of Legacy NJOY's modules that will not be implemented in NJOY21 as they are not used anymore. For more information see Section 5.2.

- Platform independent tests
- Simple execution of tests
- Easier to interact with NJOY
  - Provide scripting (i.e., Python) interface to every public component and feature
  - Provide modern interface (scripting an input "deck")
- **Easier** to process nuclear data files
  - Provide accessory tools to assist in the processing and validation of (many) nuclear data files
  - Provide methods to evaluate, process, and test nuclear data formats

### III. Flexible

- Enable multiple ways of interaction
- Enable alternative components (i.e., plugins)

### IV. Faster

- Take advantage of modern computer architectures with many CPUs
- Improve processing algorithms
- Fast memory management

### V. Maintainable

- Modularized code
- Reusable code

### 2.2 Distribution

The NJOY code (both NJOY21 and Legacy NJOY) can be found on GitHub at https://github.com/njoy. The njoy organization is owned by Jeremy Conlin and is used to host all the repositories that make up the different versions of NJOY as well as controlling who can contribute to NJOY.

In addition to the njoy organization on GitHub, we will also use the nucleardata organization to host some pieces of NJOY21. The nucleardata organization is also owned by Jeremy Conlin and is intended to be the location where one can get:

- data format specifications, and
- code to read/write data formats.

Many of the data formats that are read and created by NJOY are also used by other codes. Hosting the format specifications and read/write code routines separately from the NJOY code can help others to also read/write the same data.

NJOY or any of its components can be accessed by visiting GitHub or cloning the repository via git. There is no need to make a formal request to get or use the code thus greatly reducing the amount of time needed to get it.

### 2.2.1 Website

To provide documentation for NJOY, it's development, and how to use it, we have purchased the domain name njoy21.io. Our website is hosted on GitHub servers and can be accessed at https://www.njoy21.io. This website will continue to grow as the needs of NJOY and its users expand.

### 2.2.2 Open Source License

Beginning with NJOY2016 (and continuing with NJOY21), the code is released with an Open Source license<sup>2</sup>. This means that anyone, anywhere, can get the code without any export control restrictions. This is a big improvement over previous versions of NJOY. In many cases, our international colleagues could not obtain NJOY and were forced to write their own processing codes.

NJOY has long benefited from the contributions of external collaborators. We want to continue this relationship and facilitate the communication between NJOY developers at LANL and our colleagues around the world. Releasing NJOY without any restrictions has proven to enhance this collaboration from the initial announcement of its release.

### 2.3 Backwards Compatibility

NJOY21 will be backwards compatible with NJOY2016. That means that an input deck that runs in NJOY2016 will also run in NJOY21.

Of course, at some time, we will develop features and capabilities in NJOY21 that are not available or compatible with NJOY2016. At that time, we will have to break backwards compatibility. We do not foresee the need to break backwards compatibility for the next 5–10 years.

### 2.4 Components

In Section 5, we see that Legacy NJOY is made of of 24 different modules. The modules take as input an ENDF file and finish by writing another file (often an ENDF file). The output file can either be used by another application (e.g., ACE file used by MCNP) or used as input for another NJOY module. The Legacy NJOY modules are coupled together because they rely on the output of one to perform the calculation in another.

Similarly to Legacy NJOY, NJOY21 will be made up of many different components. The components that make up NJOY21 are decoupled from each other; that is, they don't rely on the output of one module to be able to perform their function.

The components are designed to be used in any code—not just NJOY21. This provides great flexibility because the code that is used to generate the data can be the same code that reads the data in an application code (e.g., MCNP). Alternatively, the components can be combined in different ways to provide different functionality for different needs.

Each component of NJOY21 is developed and tested independently, but can use other components to avoid the duplication of code. Keeping each component independent

<sup>&</sup>lt;sup>2</sup>3-clause BSD

makes it so that NJOY21 can be developed in several different areas at the same time, without developers interfering with each other. It also greatly reduces the compile time and testing burden of NJOY21 as most of the testing is done in each individual component; only integration tests are performed in NJOY21.

The capabilities that have been—and will be developed—are given in Section 4

### 2.5 Verification and Validation

An important aspect of ensure that NJOY21 works properly is thorough and regular testing; testing of NJOY21 as a whole, and testing of its individual components. Providing these tests to validate and verify NJOY21 is a large part of the effort required during its development.

Legacy NJOY shipped with input decks and sample outputs for 20 different scenarios. These tests provided some indication that NJOY was operating as expected. That is, does the local installation give the same answer as the reference. If one ran the tests and got a different answer, the only thing you could say was that the answer was different. There was no way to know if the reference output was correct or the new output was correct. Also, the tests were difficult to run unless NJOY was installed on Windows.

With NJOY2016 a change was made to facilitate the running of these tests. CTest is used to automate the running of the tests and works on all platforms. These tests are "integration tests" and help to identify how NJOY works as a whole.

With NJOY21 we have made testing an integral part of the development and design process; every piece of every component of NJOY21 is thoroughly tested. The code is written and designed so that each unit can be separately tested as well as tested in conjunction with other pieces. These tests are called unit tests and provide very fine grained control of every piece/unit that makes up NJOY21.

It is worth mentioning that no amount of testing can ensure that a code has zero bugs. Testing can ensure that old problems don't creep in; the tests will tell you right away if they have.

Developing the unit tests is a time consuming process. More than 50% of the development time on NJOY21 is spent developing unit tests. While this is expensive, if a problem ever enters the code, we know immediately where the problem occurs because our tests fail and tell us. Also, we *never* have to open a debugger because our tests tell us exactly what is happening. In this long run, spending the time to develop unit tests will be much more efficient than trying to find and fix bugs later.

### 2.5.1 Continuous Integration

It does no good to develop tests if they are never run. Like with NJOY2016, NJOY21 and all of it's components utilize CTest to run the tests that have been developed. To reiterate, these tests can be run on any platform on which the code is built and can be run by anyone. The end user runs the same tests the developers do and can have the same confidence that their code is correct.

To ensure that the code performs properly on all platforms, we utilize what is called continuous integration. Whenever new code is committed to a repository, the code is automatically compiled and tested in multiple configurations. We can see very quickly whether the code is working properly or not. Sometimes we will find that the code works for one compiler, but not another; continuous integration lets us know right away, we don't have to wait until a user reports that something is broken.

Now, our continuous integration is not as complete as we would like it to be. We currently run Jenkins using Amazon Web Services and have this hosted at <a href="https://jenkins.njoy21.io">https://jenkins.njoy21.io</a>. This is easily set up to test on Linux. We could test on Windows, but haven't spent much time on this. Testing on Mac is not an option with Amazon Web Services. A new option that has recently become available is Azure DevOps by Microsoft.

It really takes a dedicated person to maintain the continuous integration services that we use. I would expect about 25% of an FTE is required to do this properly.

### 3 NJOY21 in 2021

Historically, the NJOY version is related to the year in which it was released; NJOY99 was released in 1999, NJOY2012 was released in 2012, NJOY2016 was released in 2016, etc. NJOY21 breaks that trend in that the 21 in it's name stands for the 21<sup>st</sup> Century. That being said, many have asked if NJOY21 would be finished in 2021. The answer is NJOY21 will never be "finished" as the intent is to always be working on it and improving it. However, we can set some specific goals and trying to get those accomplished by 2021 is a good idea.

### Goal 1

By the end of 2021, NJOY21 will have modernized all components necessary to enable the processing of the neutron sublibrary of ENDF/B-VIII.0 to the ACE format.

In order to achieve this goal, the following Legacy NJOY modules must be modernized (given roughly in the order they should be done):

- 1. RECONR
- 2. BROADR
- 3. ACER
- 4. HEATR
- 5. MODER
- 6. PURR
- 7. GASPR

### Goal 2

NJOY21 will be able to process the neutron sublibrary into the multi-group NDI format for the ENDF/B release that comes after ENDF/B-VIII.0.

In addition to those components necessary for Goal 1, Goal 2 requires the following modules to be modernized:

- 1. GROUPR
- 2. NDIR
- 3. UNRESR

A Gantt chart<sup>3</sup> has been created to help estimate the effort needed to accomplish the goals. This is shown in Figure 1.

<sup>&</sup>lt;sup>3</sup>Last updated on 2018-11-15

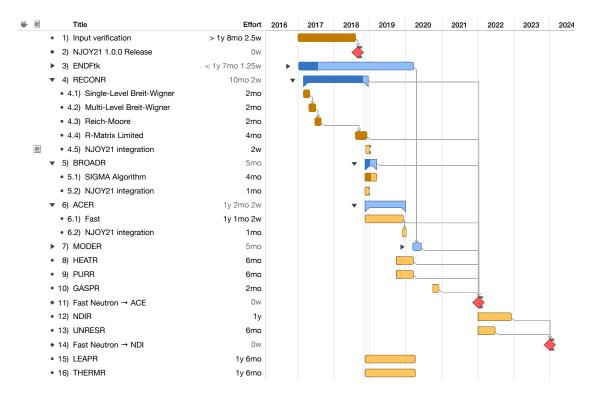


Figure 1: Gantt chart estimate of NJOY21 tasking to complete Goals 1 and 2.

- 3.1 Fiscal Year 2019
- 3.1.1 RECONR
- 3.1.2 ACER
- 3.1.3 BROADR
- 3.2 Fiscal Year 2020
- **3.2.1 MODER**
- **3.2.2 HEATR**
- 3.2.3 PURR
- 3.3 Fiscal Year 2021
- 3.3.1 GASPR

# 4 Capabilities for NJOY21

Each component in NJOY21 is designed and developed to solve a single problem, e.g., reconstructing resonances. This differs somewhat from the Legacy NJOY modules which

often did several things in addition to their main task. For example the RECONR module in NJOY2016 performs the following calculations:

- resonance reconstruction,
- energy-grid unionization,
- linearization of tabulated cross sections,
- removal of negative cross sections, and
- removal of positive cross sections below the Q-value.

While all of these pieces need to be implemented in NJOY21, they do not all have to be part of the same component.

In this section, we discuss the different capabilities that must be developed for NJOY21. We make an attempt at guessing the time required to develop each capability.

### 4.1 Resonance Reconstruction

The ENDF format currently allows several different kinds of resonance parameter formalisms:<sup>4</sup>

- Single-level Breit-Wigner (LRF=1),
- Multi-level Breit-Wigner (LRF=2),
- Reich Moore (LRF=3), and
- R-Matrix Limited (LRF=7).

The component that deals with resonance reconstruction is (naturally) njoy::resonanceReconstruction. Implementation using the Breit-Wigner and Reich Moore formalisms have been implemented and presented at the PHYSOR 2018 conference, "Resonance Reconstruction Capability in NJOY21".

Resonance reconstruction is a critical piece in the processing of nuclear data; it is typically the first processing piece that is done. Historically, the resonance reconstruction capabilities in the various nuclear data processing codes all derived from the SAMMY[2] code.<sup>5</sup> The new resonance reconstruction capability in njoy::resonanceReconstruction is perhaps only the second implementation ever.

This capability has been under development for fiscal years 2017–2018 and should be completed early fiscal year 2019. This is one of the more technically challenging capabilities that needs to be developed due to the many different formalisms that must be understood.

### 4.2 Energy-grid Linearization and Unionization

Energy-grid linearization and unionization is performed as part of the Legacy NJOY RECONR module. In NJOY21, this capability is performed in the njoy::twig component.

<sup>&</sup>lt;sup>4</sup>The ENDF format currently allows Adler-Adler formalism, but this is discouraged and hasn't been used in ENDF/B for over a decade. We don't intend to support the Adler-Adler formalism in NJOY21. <sup>5</sup>In the case of NJOY it was lifted right out of SAMMY and used in NJOY.

### 4.3 Validation of Legacy NJOY Input Values

It is not uncommon for an NJOY calculation to run for an hour and then stop because of an invalid input value. The first component of NJOY21 that is new is the validation of the input values; prior to any of NJOY21's module running, the input values are all validated. If any values are invalid, a notice is printed to the screen and the user is notified of what is expected. This has been beneficial in house as it has already found a few (minor) issues in some of the input decks we have used. This input validation is performed in the njoy::lipservice component. Note: it is not possible to ensure that all the input values are correct. It can only ensure that the values are valid, not that they are correct.

The work to validate the Legacy NJOY input values took roughly one full FTE. In Legacy NJOY, there are:

- 24 modules,
- 161 "cards", and
- 409 different input values.

Each input value is independently tested. All the input values making up a "card" are tested together. And finally, all the cards that make up a particular module are tested together. All combined there are 733 test executables with 11118 different assertions in total. This number of tests takes a long time to develop (i.e., one full year), but provides confidence that what we are attempting to do, is being done.

### 4.4 Working with Data Formats

At the heart of NJOY is nuclear data. It reads nuclear data from files and it produces nuclear data for other codes. As part of this process, it often writes intermediate data files. Every file that NJOY writes is formatted following<sup>6</sup> a given convention.

There are several different components<sup>7</sup> of NJOY21 that facilitate working with these formatted data files. The purpose of writing these components is to centralize the reading and writing of these data files. It also makes it possible to reuse these capabilities in multiple places without having to duplicate code.

As these components deal with nuclear data formats, they will be hosted under the nucleardata organization on GitHub instead of the njoy organization.

### 4.4.1 ENDF-formatted Data

Toolkit for working with ENDF-formatted files. This is done in ENDFtk or ENDF-toolkit. This toolkit is under heavy development. When a portion of the ENDF file needs to be read, section or file is developed. This will likely be moved to the nucleardata organization on GitHub as it deals with data formats.

<sup>&</sup>lt;sup>6</sup>Admittedly, this is often a loose interpretation.

<sup>&</sup>lt;sup>7</sup>These components are usually called toolkits.

### 4.4.2 ACE-formatted Data

Toolkit for working with ACE-formatted files. This is done using ACEtk or ACE-toolkit. Like ENDFtk, this toolkit is also under heavy development.

There are several different types of ACE files for different types of data:

- 1. continuous-energy and discrete-energy neutron transport data;
- 2. electron transport data;
- 3. thermal scattering or  $S(\alpha, \beta)$  data;
- 4. photonuclear transport data.
- 5. photoatomic data;
- 6. dosimetry data; and
- 7. multigroup transport data.

This list is given in (roughly) the order of interest; the order in which we intend to implement the capability of interpreting and creating that type of data.

Due to the ACE format, there are parts of ACEtk that are used regardless of the type of data. ACE data is composed of a header and four different arrays. The format of the header and arrays are the same for every type of ACE data. The difference between the types of data is in how they are interpreted. So, reading and accessing the header and arrays is the same across all the different types of ACE data.

There are two pieces of ACEtk: 1) interpretation of the ACE data, and 2) creation of the ACE data. The interpretation is what is needed for applications such as MCNP or a plotting tool to use the data; thus, the ACE data needs to *interpreted*. The creation of the ACE data occurs when NJOY takes processed data and puts it in the form required by the ACE format. Note: it is not the responsibility of ACEtk to read the data from ENDF (or some other format) to populate the ACE data. It is someone else's responsibility to read the data from ENDF and hand it to ACEtk to create the data.

The focus at the moment is on the continuous-energy neutron (or fast neutron) data. The interpretation of the continuous-energy neutron data is nearly complete; it has taken roughly a full year to get that completed. Once the interpretation is complete, we can begin to write the code that will create the ACE data tables given processed data from other components.

A parallel effort—contributing to ACEtk—is the interpretation (and eventual creation) of the electron data. This work is being done by David Dixon and his student(s) in XCP-3.

### 4.4.3 GNDS-formatted Data

### 4.4.4 NDI-formatted Data

This is a component that needs to be completed, but isn't quite high enough on the priority list to have anything done about it. This will result in a component that can read, write, and manipulate NDI-formatted data. Based on the experience of other components, I estimate this will take about 1 FTE worth of work.

### 4.5 General Utilities

There are many little utilities that are useful across many different components of NJOY21. We have created the njoy::utility to place these simple tools.

### 5 Legacy NJOY

Legacy NJOY is NJOY2016, the version of NJOY that began with the original NJOY release in 1977 and has been modified and updated since then. While still quite capable, Legacy NJOY has its limitations and cannot process data in the newest formats.

### 5.1 Maintenance Plan

In November 2017, during the Cross Section Evaluation Working Group (CSEWG) annual meeting at Brookhaven National Laboratory, it was announced that the NJOY team at Los Alamos National Laboratory would work with individuals and organizations to move their custom changes in NJOY2012 over to NJOY2016. This was done in an attempt to encourage people to move from NJOY2012 to NJOY2016. The offer was made to do this until the end of 2018, at which point, making those modifications would be up to the individual.

In addition, LANL committed to back-porting all features and bug fixes from NJOY2016 to NJOY2012. In reality, the back porting was performed by Skip Kahler under contract from the International Atomic Energy Agency, rather than LANL. Nevertheless, the codebase for NJOY2016 and NJOY2012 remain the same.

As a result of this announcement, the NJOY team has made several updates to NJOY2016 that had previously only been in private use by individuals at different organizations. Those contributions have come from:

- International Atomic Energy Agency (IAEA), Nuclear Data Section, Vienna, Austria; and
- Polytechnique de Montréal, Montreal, Canada.

At the 2018 meeting of the Reactor Physics and Shielding Division of the American Nuclear Society [3], it was announced that NJOY2016 is officially deprecated. This means that no new features are being added to NJOY2016, only bug fixes are being made. NJOY users are encouraged to use NJOY21 for all their production needs. Since NJOY21 is backwards compatible with NJOY2016, input decks should be useable without any change in NJOY21.

We intend to continue to provide bug fixes to NJOY2016 until the next release of the ENDF/B library; This will likely take place in 2023 or 2024.

### 5.2 Legacy NJOY Modules

Legacy NJOY consists of 24 different modules; each module provides different functionality. The functionality of most of the modules will need to be modernized for NJOY21; some of them (e.g., WIMSR, CCCCR) may not ever get modernized as they are not in modern use—although the number that will not get modernized is few. The modules will get updated as demand requires.

Provided here is a short description of each of these modules (taken from *The NJOY Nuclear Data Processing System, Version 2016*, Chapter 1.

- NJOY directs the flow of data through the other modules. Subsidiary modules for locale, ENDF formats, physics constants, utility routines, and math routines are grouped with the NJOY module for descriptive purposes.
- **RECONR** reconstructs point-wise (energy-dependent) cross sections from ENDF resonance parameters and interpolation schemes.
- **BROADR** Doppler-broadens and thins point-wise cross sections.
- **UNRESR** computes effective self-shielded point-wise cross sections in the unresolved energy range.
- **HEATR** generates point-wise heat production cross sections (neutron KERMA factors) and radiation damage production cross sections.
- **THERMR** produces cross sections and energy-to-energy matrices for free or bound scatterers in the thermal energy range.
- **GROUPR** generates self-shielded multigroup cross sections, group-to-group scattering matrices, photon production matrices, and charged-particle multigroup cross sections from point-wise input.
- **GAMINR** calculates multigroup photoatomic cross sections, photon KERMA factors, and group-to-group photon scattering matrices.
- **ERRORR** computes multigroup covariance matrices from point-wise covariance data.
- **COVR** reads the output of ERRORR and performs covariance plotting and output formatting operations.
- MODER converts ENDF "tapes" back and forth between formatted (that is, ASCII) and blocked binary modes.
- DTFR formats multigroup data for transport codes that use formats based on the DTF-IV code.
- CCCCR formats multigroup data for the CCCC standard files ISOTXS, BRKOXS, and DLAYXS.
- MATXSR formats multigroup data for the newer MATXS cross-section interface file, which works with the TRANSX code to make libraries for many particle transport codes.
- **RESXSR** prepares point-wise cross sections in a CCCC-like format for thermal flux calculators.
- ACER prepares libraries in ACE format for the Los Alamos continuous-energy Monte Carlo MCNP and MCNPX codes. The ACER module is supported by subsidiary modules for the different classes of the ACE format.
- **POWR** prepares libraries for the EPRI-CELL and EPRI-CPM codes.
- WIMSR prepares libraries for the thermal reactor assembly codes WIMS-D and WIMS-E.
- PLOTR makes plots of cross sections and perspective plots of distributions for both point-wise and multigroup data by generating input for the VIEWR module.
- **VIEWR** converts plotting files produced by the other modules into high-quality color Postscript plots.
- MIXR is used to combine cross sections into elements or mixtures, mainly for plotting.
- **PURR** is used to prepare unresolved-region probability tables for the MCNP continuous-energy Monte Carlo code.

- **LEAPR** produces thermal scattering data in ENDF-6 File 7 format that can be processed using the THERMR module.
- **GASPR** generates gas-production cross sections in the point-wise PENDF format from basic ENDF cross sections.

### References

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- [9] D.E. Cullen. Program SIGMA1 (version 79-1): Doppler broaden evaluated cross sections in the evaluated nuclear data file/version B (ENDF/B) format. Tech. rep. United States, Oct. 1979. DOI: 10.2172/5254306.

### A Fiscal Year 2018

### A.1 Supporting ENDF/B-VIII.0

Much of FY2018 was spent in preparation for ENDF/B-VIII.0. There were a number of updates to NJOY2016 that were made to support the correct processing of ENDF/B-VIII.0 [5].

Each release of the ENDF/B library often results in the introduction of new data formats in the ENDF-6 format. With ENDF/B-VIII.0, new formats were added for allowing tabulated fission energy release components, to allow for sub-actinide fission and non-neutron induced fission, and to add fission neutron and gamma emission probabilities. Processing codes must be adapted to ensure that they are capable of using these new data, or at the very least understand the new formats. NJOY2016 is no exception to this.

In addition to format changes, a new evaluated nuclear data library also tends to push the limits of the processing codes leading to a number of fixes and updates to correct problems that were uncovered while processing the beta releases and final release of ENDF/B-VIII.0:

- updates to ACER for plot generation and thermal scattering data formatting;
- updates to ERRORR for covariance processing;
- updates to LEAPR for generating thermal scattering data;
- updates to PURR for unresolved resonance probability tables;
- updates to THERMR for thermal scattering data;
- integration of an NJOY2012 update file from the IAEA.

More information about the updates to NJOY2016 are given in the following reports:

- NJOY2016 updates for ENDF/B-VIII.0,
- New fission heating capabilities in the NJOY2016 HEATR module, and
- "Updating NJOY's HEATR Module for ENDF/B-VIII.0".

# A.2 Development of Resonance Reconstruction Capabilities for the R-Matrix Limited Format

In FY2017, resonance reconstruction capabilities were developed for the Single-level Breit Wigner, Multi-level Breit Wigner, and Reich-Moore formats. These make up the resonanceReconstruction component of NJOY21. In FY2018, the *R*-Matrix Limited (RML) format was added. The RML format is the most complicated of all of the resonance formalisms.

The integration of resonanceReconstruction into NJOY21 will be performed in FY2019. (See Section A.5.)

### A.3 Implementation of Doppler Broadening Capabilities

Doppler broadening capabilities have been developed for NJOY21. This used the same algorithm as used in the SIGMA1 [9] code in PREPRO. Like with the resonance reconstruc-

tion capabilities, these have not yet been integrated into NJOY21, but will be integrated in FY2019.

### A.4 Generalized Nuclear Database Structure (GNDS)

We have been active participants in the development of GNDS. A major part of this is participating in Subgroup 43 of the Working Party on International Nuclear Data Evaluation Co-operation (WPEC), for which Jeremy Conlin serves as Co-Chair. Subgroup 43 is tasked with developing the infrastructure to support and facilitate the use of GNDS by a wider audience. As a result of this on-going subgroup, more institutions are adopting GNDS and developing capabilities to work with that format.

### A.5 FY2019 Plans

We have big plans for NJOY21 in FY2019. We have spent several years preparing components in the background; in FY2019, we will integrate many of those components to replace the first legacy modules with fully modern components.

### A.5.1 Integration of Modern RECONR into NJOY21

The resonance reconstruction capabilities were completed in FY2017 and FY2018. In FY2019, we will combine the resonance reconstruction capabilities along with:

- cross section linearization, and
- energy grid unionization.

With these components in place, the legacy RECONR module will be the first one replaced with entirely modern components in NJOY21.

### A.5.2 Integration of Modern BROADR into NJOY21

With the implementation of the SIGMA1 algorithm for Doppler broadening completed in FY2018, we are ready to integrate this into NJOY21 in FY2019. This would replace the legacy BROADR module and follows nicely after the modernization of the RECONR module.

### A.5.3 Implement and Integrate ACER for Fast Neutrons into NJOY21

This is the most ambitious goal for FY2019. It requires a lot of work on several different components, including:

### - ENDFtk

This would require reading data from the following ENDF files:

MF=1 General information including fission nubar and fission energy release;

MF=3 reaction cross sections;

MF=4-6 secondary angular and energy distributions;

MF=12 photon production yields;

MF=13 photon production cross sections;

MF=14-15 secondary photon angular and energy distributions.

### - ACEtk

The building of an ACE file is challenging due to the complicated bookkeeping necessary to properly index the various arrays in the ACE format. In addition, some data processing is performed by the legacy ACER module to prevent overestimation of the scattering cross section at low energies.

This will work will take the majority of the year to complete. There is a risk of this not being completed due to the amount of work needed exceeding the estimate. Nevertheless, we are working to complete this work in FY2019.

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NCSP Element and Subtasks: AM2, 3, 5, 6, 7

**Task Titles:** 

AM2 Multiphysics Methods for the Simulation of Criticality Accidents

AM3 Slide Rule Application

AM5 Proposed Benchmark Intercomparison Study

AM6 Proposed 1-D Multipoint Analytical Benchmark Comparison
AM7 Technical Data for the Pitzer Formulation of Solution Compositions

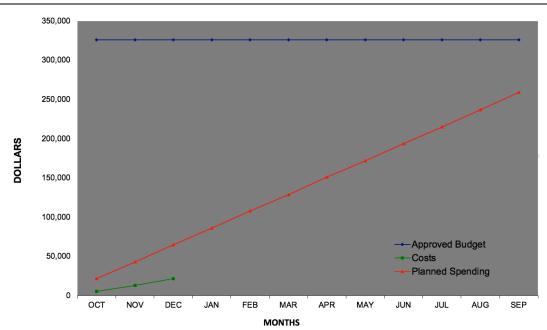
**M&O Contractor Name:** Lawrence Livermore National Laboratory

**Point of Contact Name:** David Heinrichs **Point of Contact Phone:** (925) 424-5679

Reference: B&R DP0909010

Date of Report: January 25, 2019





- Carryover into FY 2019 = \$45,203
- 2. Approved FY 2019 Budget = \$326,203 (includes carryover)
- 3. Actual spending for 1st Quarter FY 2019 = \$22,055
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$
- 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$
- 7. Projected carryover into FY 2020 = \$67,203 (21%)

### **MAJOR ACCOMPLISHMENTS**

- 1. Implemented new ENDF/B-VIII.0 data in COG representing the energy dependent number vs. probability 'multiplicity data' for prompt fission neutrons and photons (AM2).
- 2. Provided TART2012 and TART2016 (original) software to Marc Klasky, LANL, Applied Modern Physics (P-21), to assist LANL in their development of analytical methods to calculate negative alpha eigenvalues (AM2).
- 3. Implemented parallel processing for the Criticality Detector Variance Reduction (CritDetVR) option in COG to enable more efficient (hybrid) calculations of far field doses with variance reduction techniques and unbiased criticality (source) calculations (AM3).
- 4. Provided high-precision COG benchmark results using ENDF/B-VII.1 to Isabelle Duhamel (IRSN) for a total of 1,942 ICSBEP benchmark cases for inclusion in the *Benchmark Inter-comparison Study* (AM5) as follows:

PU: 526 U233: 194 MIX: 28 HEU: 762 IEU: 188 LEU: 244

- Submitted LLNL-ABS-763661, Expanded COG Criticality Validation Suite, to the International Conference on Mathematics and Computational Methods applied to Nuclear Science and Engineering (M&C 2019) (AM5).
- LLNL Supply Chain Management completed a contract with Dr. Barry Ganapol, U. Arizona, to develop the proposed 1-D multipoint analytical benchmark (AM6).
- LLNL (Catherine Percher), LANL (Jen Alwin) and Chuck Weber (ORNL) participated in a kick-off teleconference in December 2018 to determine the scope of the technical data needs (AM7).

### **LLNL AM Milestones:**

STATUS (copy color code and paste below in 'STATUS' field)

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Complete	On Schedule	Behind Schedule	Missed Milestone		

QUARTER	MILESTONE	STATUS	COMMENTS
Q1	Provide status on LLNL AM activities in NCSP Quarterly Progress Reports (AM2, AM3, AM5, AM6, AM7).		
Q2	Provide status on LLNL AM activities in NCSP Quarterly Progress Reports (AM2, AM3, AM5, AM6, AM7).		
Q3	Provide status on LLNL AM activities in NCSP Quarterly Progress Reports (AM2, AM3, AM5, AM6, AM7).		
Q4	Provide status on LLNL AM activities in NCSP Quarterly Progress Reports (AM2, AM3, AM5, AM6, AM7).		

### **Task Titles:**

AM2 Multi-Physics Methods for Simulation of Criticality Excursions

AM3 Slide Rule Application

AM5 Proposed Benchmark Intercomparison Study

AM6 Proposed 1-D Multipoint Analytical Benchmark Comparison

AM7 Technical Data for the Pitzer Formulation of Solution Compositions to Include Uranium/Plutonium Solutions with Selected Admixed Absorbers

NCSP Element and Subtask: ORNL – AM1, 2, 3, 6, 9, 10, 11, 13, 14, 15, 16

Task Titles: See last page
M&O Contractor Name: ORNL
Point of Contact Name: Doug Bowen
Point of Contact Phone: (865) 576-0315

Reference: DP0909010/ORNL Date of Report: January 20, 2019

### **BUDGET**

# FY19 Analytical Methods 3,000 2,500 2,000 1,000 500 Oct Nov Dec Jan Feb Mar Apr May Jun Jul Aug Sep Approved Budget Planned Spending

- 1. Carryover into FY 2019 = \$301K
- 2. Approved FY 2019 Budget = \$2521k (includes carryover)
- 3. Actual spending for 1st Quarter FY 2019 = \$388K
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$
- 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$
- 7. Projected carryover into FY 2020 = \$

### **MAJOR ACCOMPLISHMENTS**

### AM1 – Distribution of available and newly packaged software

- o Distributed 574 software packages and updated 6 software packages.
- o 94 SCALE, 328 MCNP®, and 0 COG packages distributed.
- RSICC quarterly report issued.

# AM2 - SCALE/KENO/TSUNAMI Maintenance and Support/Cross-Section and Generation/Modernization

- Tasks were initiated to increase the output capabilities and robustness of the new high-performance Monte Carlo transport kernel, Shift, called from within SCALE's Criticality Safety Analysis Sequence (CSAS). Within SCALE, we have begun the process of integrating Shift and deprecating the older KENO and MONACO Monte Carlo modules.
  - Shift is supported by DOE's Exascale Computing Projection (ECP) and through those funding sources will become a next generation Monte Carlo platform for next generation machines. However, in order to smoothly transition over the next 3-5 years, the user-friendliness of CSAS-Shift for the average criticality user, in areas such as geometry checking and error reporting, requires additional investments. After the first round of user testing during FY19 Q1, a list of 77 additional requests was compiled and prioritized. Most of the requests require access to additional interfaces within Shift for accurate and useful error reporting. Some issues with the complex geometry were also identified. Efforts in Q2 and Q3 will continue to iterate on CSAS-Shift in order to improve the user experience for the 6.3.0 release.
- Testing was performed of a recent implementation of the Iterated Fission Probability Monte Carlo sensitivity method within Shift. Some recent staff changes have required new, junior staff become involved in sensitivity space in order to maintain this capability.
- SCALE testing infrastructure updates were performed to make it easier to run additional SCALE test suites on demand or automatically according to a schedule. SCALE currently runs ~5000 tests on Windows, Mac, and Linux consuming ~30 CPU-hours for every merge of developer changes into the main repository. However, these tests are intended to identify developer error and regression and not necessarily the real performance of SCALE for a standard benchmark. Actual performance is best determined through validation, such as with the VALID archive of SCALE criticality models. The SCALE testing infrastructure now supports running test suites like VALID with a push-

### NCSP Quarterly Progress Report (FY-2019 Q1) button request from the main project site, accessible to all developers. In FY19 Q2, the actual VALID suite will be uploaded and automatic, scheduled runs will be created, in addition to the push-button capability made available in Q1. AM3 - AMPX Maintenance and Modernization The two lead AMPX developers attended the annual CSEWG and NDAG meetings hosted at BNL in November, contributing invaluable technical discussions, including presentations about last year's AMPX improvements, as well as the processing and subsequent verification and validation testing of last year's ENDF-VIII.0 release. Modifications to the AMPX source code were made to support external linking against the LAPACK wrappers in SCALE; this allowed for the NCSP supported code SAMMY to have easy access to all of the complex linear algebra solver routines included in the SCALE math utilities package. Further, this infrastructure improvement in AMPX provides a template for future improvements in code clarity and integration between AMPX and SAMMY. In connection with an NRC project the AMPX code broaden, used to Doppler broaden point-wise cross section data, we converted the code that broadens a single energy point using the Solbrig kernel approximation. In addition we implemented the same thinning mechanism for the broadened data as previously done in the Fortran code. In addition to passing all existing unit test, we also compare results of the old version and the new version of broaden, using all nuclides from the ENDF/VIII.0 library. AM6 – SlideRule Application No work has been performed on this IRSN-led task in Q1. AM9 - Sensitivity/Uncertainty Comparison Study with a Focus on Upper Subcritical Limits ORNL is behind schedule, memo report on ORNL results in progress. Path forward is to compare results with those from LANL and IRSN. AM10 - Proposed Benchmark Intercomparison Study This task is a benchmark comparison with LLNL, LANL, and IRSN, to be coordinated by IRSN. IRSN has not provided or solicited any details regarding the details of this task, so no work was performed at ORNL in Q1 supporting AM10. AM11 – Proposed 1-D Multipoint Analytical Benchmark Intercomparison No work has been performed on this task in Q1. Awaiting kickoff meeting after LLNL has set up a contract with the University of Arizona. AM13 - Nuclear Data and Cross Section Testing Using ENDF/B-VIII.0

## NCSP Quarterly Progress Report (FY-2019 Q1) We have successfully created both multigroup and continuous energy cross section libraries based on ENDF/B-VIII.0 release. We started with what was in the software distribution package and built SCALE (on Linux and with the help of Cihangir on Macs), which includes AMPX modules, on both Linux and Mac platforms. We then used Exsite and example templates (with modifications to fit our system) on both Macs and Windows machines to create input files needed to process the ENDF/B-VIII.0 evaluations. The inputs that were created on Macs worked fine and were used to create the continuous energy and multigroup cross section libraries. However, there were issues running test cases with some of the nuclides using these libraries. A meeting was held with Doro to determine the cause and remedy the issues (primarily wrong atomic weight ratios). After the corrections, except for some new thermal kernel cases (these will be further investigated but are lower probability), all test cases ran successfully. The inputs that were created on Windows machine had problems with either nuclide IDs or in some cases were missing parts of the input. We believe that is because the input generator was not tested on Windows and has issues. Although we used identical templates, the inputs came out different. Another student has independently run the test cases to confirm the successful library generation. We are now in the stage to run verification and validation problems and perform comparisons. AM14 - Development and Addition of Continuous-Energy Sensitivity Data Files to SCALE's **VALID Library** Work identifying optimized calculation parameters for CE TSUNAMI calculations was focused in low-enriched solution experiments in Q1. The complete set of 19 experiments is nearly complete, with only a few remaining challenges. Refinements have been made to both the TSUNAMI calculations and the reference (direct perturbation) calculations, and good agreement has been achieved in most cases. Work will continue in quarters 2 and 3 focusing on identifying optimal parameter sets for low-enriched pin array systems. The documentation to support adding these models to the Verified, Archived Library of Inputs and Data (VALID) will also be generated. Additionally, the student working on AM14 has undertaken a significant validation study for deuterium-moderated systems, examining all ICSBEP benchmarks involving heavy water or deuterium moderated/reflected systems. This a total of 89 cases and includes experiments in all neutron energy ranges (thermal, intermediate, and fast), as well as varying levels of uranium enrichment and fissile material compositions. Sixteen evaluations containing 89 cases that utilize deuterium as the moderator/reflector were modeled using SCALE 6.2.3 (continuous energy and multigroup), MCNP 6.1.b (continuous energy), and SERPENT 2 (continuous energy), with the ENDF/B-VII.1 and -VII libraries. Depending on the complexities of the geometries, KENO-V.a or -VI was

# NCSP Quarterly Progress Report (FY-2019 Q1) used to develop specific models in SCALE 6.2.3. C/E ratios were calculated for each case and compared to each other to identify possible trends. Results indicate that the combination of codes and libraries tend to overestimate LEU, metal, and thermal systems, while underestimating HEU, solution, compound, fast, and intermediate systems. The average C/E values indicate that the bias for a variety of differing systems is less $3.0\%\Delta k$ with an average bias of $0.77\%\Delta k$ . Sixty-five of the 89 experiments had a C/E difference of less than 500 pcm. There is a noticeable decrease in the C/E ratios as the neutron energy moves from the thermal to the intermediate spectrum; results in the fast region are generally close to unity. The results establish a foundation for examining or developing insight into any or possible problems/anomalies with the codes, libraries, or experimental setups for deuterium systems. The next steps are to develop models and documentation for possible inclusion in VALID. Most of this work was performed in Q3 and Q4 of FY18 but was completed in Q1 of FY19. Draft documentation for publication in a journal was also generated in Q1. AM15 - The Effects of Temperature on the Propagation of Nuclear Data Uncertainty in Nuclear Criticality Safety Calculations This task is accepted work to fund a student PHD project at MIT. A contract with MIT is currently in development and work will commence following implementation of the contract, hopefully in Q2. A student has been identified and the hope is that this student will someday work in the NCSP Nuclear Data program. AM16 - Technical Data for the Pitzer Formulation of Solution Compositions to Include Uranium/Plutonium Solutions with Selected Admixed Absorbers Funds were received a few days before Thanksgiving, and accounts were set up and ready for use the week after Thanksgiving. The month of December was focused on getting started and two items are worthy of note: 1) We held a telecon with collaborators Catherine Percher (LLNL) and Jennifer Alwin (LANL) to scope out tasks, communications, and collaboration. 2) I went through old files from 2003-2005 to identify data sets and procedures that were used when the Pitzer model work was initiated; even though old, files appear to be completely accessible and sufficiently documented.

## **ORNL AM Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

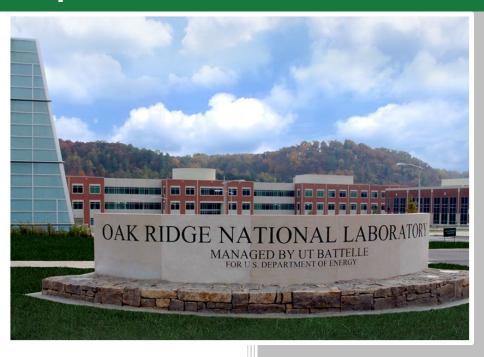
QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Continue distribution of available and newly packaged software to the NCS community requesters (at no direct cost to them) and provide distribution totals quarterly. (AM1)		
	Provide status reports on ORNL participation in US and International Analytical Methods collaborations and provide brief trip summary report to NCSP Manager on items of NCSP interest. (AM2, AM3)		
	Provide status on ORNL AM activities in NCSP Quarterly Progress Reports. (AM1, AM2, AM3, AM6, AM9, AM10, AM11, AM13, AM14, AM15, AM16)		See above
Q2	Continue distribution of available and newly packaged software to the NCS community requesters (at no direct cost to them) and provide distribution totals quarterly. (AM1)		
	Provide status reports on ORNL participation in US and International Analytical Methods collaborations and provide brief trip summary report to NCSP Manager on items of NCSP interest. (AM2, AM3)		
	Provide status on ORNL AM activities in NCSP Quarterly Progress Reports. (AM1, AM2, AM3, AM6, AM9, AM10, AM11, AM13, AM14, AM15, AM16)		
	Issue an annual SCALE maintenance report to the NCSP Manager. (AM2)		
Q3	Continue distribution of available and newly packaged software to the NCS community requesters (at no direct cost to them) and provide distribution totals quarterly. (AM1)		
	Provide status reports on ORNL participation in US and International Analytical Methods collaborations and provide brief trip		

	summary report to NCSP Manager on items of NCSP interest. (AM2, AM3)  Provide status on ORNL AM activities in NCSP Quarterly Progress Reports. (AM1, AM2, AM3, AM6, AM9, AM10, AM11, AM13, AM14, AM15, AM16)	
Q4	Continue distribution of available and newly packaged software to the NCS community requesters (at no direct cost to them) and provide distribution totals quarterly. (AM1)	
	Provide status reports on ORNL participation in US and International Analytical Methods collaborations and provide brief trip summary report to NCSP Manager on items of NCSP interest. (AM2, AM3)	
	Provide status on ORNL AM activities in NCSP Quarterly Progress Reports. (AM1, AM2, AM3, AM6, AM9, AM10, AM11, AM13, AM14, AM15, AM16)	
	Publish annual newsletter to users to communicate software updates, user notices, generic technical advice, and training course announcements. (AM2)	
	Document AMPX modernization and technical support for SCALE CE, multigroup, and covariance libraries and report status annually to the NCSP Manager. (AM3)	

#### **Task Titles:**

AM1 Radiation Safety Information Computational Center (RSICC) AM2 SCALE/KENO/TSUNAMI Maintenance and Support/Cross-Section and Generation/Modernization **AMPX Maintenance and Modernization** AM3 Slide Rule Application AM6 AM9 Sensitivity/Uncertainty Comparison Study with a Focus on Upper Subcritical Limits Proposed Benchmark Intercomparison Study Proposed 1-D Multipoint Analytical Benchmark Intercomparison Nuclear Data and Cross Section Testing Using ENDF/B-VIII.0 Development and Addition of Continuous-Energy Sensitivity Data Files to SCALE's VALID Library AM14 The Effects of Temperature on the Propagation of Nuclear Data Uncertainty in Nuclear Criticality Safety Calculations Technical Data for the Pitzer Formulation of Solution Compositions to Include Uranium/Plutonium Solutions with Selected Admixed Absorbers

# NCSP Analytical Methods Subtask 3: AMPX Development and Maintenance



Dorothea Wiarda Andrew M. Holcomb Mark L. Williams B. J. Marshall

December 2018

Not for public release.



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## ORNL/LTR-2018/1074

## Reactor and Nuclear Systems Division

# NCSP ANALYTICAL METHODS SUBTASK 3: AMPX DEVELOPMENT AND MAINTENANCE

Dorothea Wiarda Andrew M. Holcomb Mark L. Williams B. J. Marshall

December 11, 2018

Prepared for the National Nuclear Security Administration Nuclear Criticality Safety Program

Prepared by
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UT-BATTELLE, LLC
for the
DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

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	ENDF Releases and SCALE Libraries	
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#### 1. INTRODUCTION

The objective of the US Department of Energy (DOE) Nuclear Criticality Safety Program (NCSP) Analytical Methods program element is to sustain state-of-the-art radiation transport modeling capabilities and the expertise necessary to develop, maintain, and disseminate the requisite analytical tools and data libraries in a manner that is responsive to the needs of those responsible for developing, implementing, and maintaining criticality safety. To this end, the objective of the AMPX<sup>1</sup> Development and Maintenance Subtask is to ensure that the AMPX cross section processing system is available to prepare cross section and covariance libraries needed by SCALE<sup>2</sup> and other radiation transport packages to support criticality safety analyses of systems with fissionable material. Moreover, the task ensures that the cross section processing software is current with the Evaluated Nuclear Data File (ENDF/B)<sup>3</sup> formats and procedures for disseminating evaluated cross section data provided through new measurement and evaluation work efforts. The AMPX subtask provides for the production of data libraries needed for criticality safety analyses. As such, the task provides a bridge between nuclear data evaluations and radiation transport software. Without the AMPX cross section processing task, the ability to maintain and update the SCALE nuclear data libraries (cross section and covariance data) would be hindered. Therefore, the AMPX Development and Maintenance Subtask ensures that SCALE is up to date with the latest cross section data for supporting criticality safety analyses. This report summarizes the FY 2018 AMPX development and maintenance activities that have been performed in support of the NCSP. Specifically, the report summarizes the AMPX code system updates and modernization accomplishments that have been made to the software package. This report satisfies the following reporting milestone in the NCSP FY17-18 Five Year Plan:

Document AMPX modernization and technical support for SCALE CE, multigroup, and covariance libraries and report status annually to the NCSP Manager (AM3: Q2)

## 2. ENDF RELEASES AND SCALE LIBRARIES

A new version of the ENDF library (ENDF/B-VIII.0) was released February 2, 2018.<sup>4</sup> Prior to the release, Oak Ridge National Laboratory (ORNL) was involved in ongoing testing of the covariance data, as well as the generation and testing of the new library. Initial results were presented at the annual Cross Section Evaluation Working Group (CSEWG) meeting in November 2017.<sup>5,6</sup> Because there was a format change in the ENDF libraries just prior to the release, a change in AMPX was necessary. The format change allows ENDF libraries to provide not only the average multiplicity of fission neutrons, but also the probabilities for getting 0, 1, etc., neutrons after fission. While the total multiplicity is still given and is still used by AMPX, a new flag was introduced into the ENDF format. Due to the rigid nature of the current ENDF format, AMPX cannot just ignore the flag. Instead, AMPX must read the flag and, depending on its value, ignore certain records in the file. In order to process the ENDF/B-VIII.0 library, AMPX was changed accordingly. While the update in the format and the subsequent update in AMPX was not ready in time to be included into the SCALE 6.2.3 release, a patch was generated and made available via e-mail to interested parties.

The physics of nuclear reactions changes for low-incident energy, especially if the target nuclide is in a liquid or solid. For this reason, ENDF contains cross section data for neutron reactions in the thermal range for certain materials such as <sup>1</sup>H in H<sub>2</sub>O or Zr in ZrH. To make the data available to SCALE, the thermal data are combined with cross section data that cover the remaining energy range. For example, <sup>1</sup>H in H<sub>2</sub>O is combined with cross section data for the stationary nuclide for <sup>1</sup>H, and this combination is given a unique SCALE ID of 1001. In a similar fashion, <sup>90</sup>Zr for the stationary nuclide is combined with ZrH cross section data and given a unique SCALE ID of 1040090, <sup>91</sup>Zr for the stationary nuclide is combined

with ZrH cross section data and given a unique SCALE ID of 1040091, and so on. SCALE includes an internal list, the Standard Composition Library, of nuclides and human readable names that can be used if constructing SCALE input. Due to renewed interest in these thermal cross section data, ENDF/B-VIII.0 has many more of these moderator data than included in previous releases. To use these data, the Standard Composition Library was updated with new SCALE ID numbers for these moderator data. However, this is not an automated process, as there is not a good recipe for assigning the SCALE ID. This is because the ENDF ID assigned to the moderators is not unique across ENDF releases and different cross section libraries. In addition, the ENDF formatted file contains Z and A values, but these are not always set correctly. Therefore, the numbers must be assigned by hand before the new data can be used in SCALE. The updated Standard Composition Library will be available in the upcoming SCALE beta release.

As described above, ENDF/B-VIII.0-beta libraries were generated for testing in SCALE. Preliminary testing was performed on these libraries and reported at 2017 the Nuclear Criticality Safety Division (NCSD) meeting in Carlsbad, New Mexico,<sup>7</sup> and at the NCSP Technical Program Review (TPR) meeting. In conjunction with work funded by the US Nuclear Regulatory Commission (NRC), new data libraries were produced to be released with the upcoming SCALE 6.3 beta release. These libraries include a new 252 neutron group library primarily for use in thermal systems, a 302 neutron group library for use in fast systems, a 1597 neutron group library, as well as continuous energy libraries. A new 56 neutron group covariance library was also produced, along with perturbation factors. All of these libraries were tested extensively to ensure that they work well with SCALE.

In addition, new multigroup and continuous energy libraries for ENDF/B-VII.1 containing the fix for the probability tables discussed in a previous annual report<sup>8</sup> will also be included in the upcoming SCALE 6.3 beta release.

#### 3. AMPX TRAINING

AMPX has traditionally been distributed only on LINUX and MacOS. However, it would be advantageous to be able to run AMPX on Windows machines, especially since SCALE training is usually given using Windows machines. In preparation for AMPX training, work commenced on compiling and running AMPX on Windows. The primary cause of failure occurred when reading ASCII formatted files such as ENDF data. The ENDF files are distributed by the National Nuclear Data Center (NNDC)<sup>3</sup> and mostly have LINUX and MAC style line breaks. In order to make these files readable in AMPX on Windows, files must be opened with a special flag. This flag is of no consequence on Linux and MAC. This allows AMPX to be compiled and run on Windows. Some minor numerical differences between the results on Linux and Windows cause the AMPX regression tests to fail, but the differences are small enough that the code can be used for training purposes. Work continues on investigation to resolve those differences. As part of the SCALE user group meeting, a half-day hands-on tutorial for was presented AMPX using the updated Windows release and updated example ENDF files and libraries distributed with AMPX. With sponsorship from NRC, additional AMPX training sessions are planned in the future.

# 4. GENERALIZED NUCLEAR DATABASE STRUCTURE (GNDS)

The ENDF community is in the process of developing a new ENDF format, Generalized Nuclear Database Structure (GNDS). The original plan was to release the ENDF/B-VIII.0 library in the old and new formats. Unfortunately, the format is not fully specified, so ENDF/B-VIII.0 was not yet released in GNDS format, and the original Working Party on International Nuclear Data Evaluation Co-operation (WPEC) subgroup (SG-38) has not finished its final report. However, two new subgroups have been formed. One is the expert group (EG) that will govern the format (EG-GNDS), and another subgroup on infrastructure (SG-43) is to develop an application program interface (API) and some physics tests based

on the API for GNDS. Both groups met at WPEC meeting in Paris in May. A report on the progress of GNDS support in AMPX was given in both of those subgroup neetings. 10,11

Work has progressed on the capability of the AMPX code to read the GNDS data files with a focus on reading the covariance data for resonance parameters. AMPX can now read all cross section covariance data and resonance parameters covariance matrices from GNDS. The covariance data from ENDF formatted files and GNDS formatted files were processed, and the results were compared. Differences were traced back to inconsistencies in the FUDGE code that was developed by Lawrence Livermore National Laboratory (LLNL). The results were discussed with the developers of FUDGE. Once the updated version of FUDGE is available, the comparison will continue. The support of GNDS in AMPX is funded by NCSP and NRC. Funding from NCSP was mainly used to add the covariance processing and to compare results between processing from GNDS and ENDF formatted files.

In addition, we started work on processing the kinematic data and read the elastic and discrete inelastic kinematic data. Comparison of the results is ongoing.

It is anticipated that the code developed for GNDS processing is going to be released with the upcoming SCALE 6.3 beta release. The code will not be available in the pre-compiled binaries but will be available for testing and compiling by interested users.

In addition, we anticipate incorporating the AMPX ENDF reading routine into SAMMY<sup>12</sup>, which will give SAMMY the ability to read and write ENDF files in GNDS as well as in the old format. It is our intent to share more code between AMPX and SAMMY in order to avoid code duplication. Currently AMPX already uses SAMRML from SAMMY to generate derivatives of the cross-section data with respect to the resonance parameters. Switching to the full version of SAMMY for this task, as well as for calculating cross section data in the resolved range, will allow us to take full advantage of new SAMMY features.

## 5. SUMMARY

In summary, the NCSP FY2018 AMPX Maintenance and Modernization funds were used to test ENDF/B-VIII.0 libraries before and after final release of the library for transport and covariance libraries. In addition, new multigroup and continuous energy libraries based on ENDF/B-VIII.0 have been created for distribution with the next SCALE 6.3 beta. In addition, AMPX was updated to allow compilation on Windows platforms in preparation for AMPX training. To support the new GNDS format, code development continued to enable AMPX to process GNDS-formatted files. It is anticipated that the GNDS reading and writing routines developed for AMPX will also be used in SAMMY in order to avoid duplication of effort.

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- 3. "Evaluated Nuclear Data File (ENDF)," Database Version VII.0, <a href="http://www.nndc.bnl.gov/endf/index.html">http://www.nndc.bnl.gov/endf/index.html</a>, National Nuclear Data Center, Brookhaven National Laboratory Associated Universities, Inc., Upton, Long Island, New York.

- 4. D. A. Brown, et al., "ENDF/B-VIII.0: The 8<sup>th</sup> major release of the nuclear reaction data library with CIELO-project cross sections, new standards and thermal scattering data," *Nucl. Data Sheets* **148**(2018)1.
- M. Williams, D. Wiarda, B. J. Marshall, and A. Holcomb, "ENDF/B-VIII-beta Data Testing at ORNL," 2017 CSEWG Meeting, Brookhaven National Laboratory, November 6–9, 2017, <a href="https://indico.bnl.gov/event/3580/contributions/10511/attachments/9416/11516/DataTesting\_CSEWG">https://indico.bnl.gov/event/3580/contributions/10511/attachments/9416/11516/DataTesting\_CSEWG</a>
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- 9. C. M. Mattoon, B. R. Beck, N. R. Patel, N. C. Summers, and G. W. Hedstrom, "Generalized Nuclear Data: A New Structure (with Supporting Infrastructure) for Handling Nuclear Data," *Nucl. Data Sheets* **113**(12), 3145–3171 (2012).
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- 12. N. M. Larson, "Updated User's Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations," ORNL/TM-9179/R6 (July 2003).

NCSP Element and Subtasks: IPD1, 2, 4

Task Titles:

IPD1 Conduct ICSBEP for Benchmarks listed in Appendix C of the 5-Year Plan and publish annual

revision to the Handbook

IPD2 Maintain the NCSP Website and Systems

IPD4 Benchmark Evaluation of Hot Box, LLNL Historical Critical Configurations at High Temperature

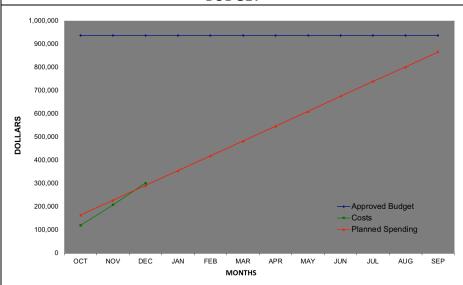
**M&O Contractor Name:** Lawrence Livermore National Laboratory

**Point of Contact Name:** David Heinrichs **Point of Contact Phone:** (925) 424-5679

Reference: B&R DP0909010

Date of Report: January 25, 2019

#### BUDGET



- Carryover into FY 2019 = \$102.907
- 2. Approved FY 2019 Budget = \$935,907 (includes carryover)
- Actual spending for 1<sup>st</sup> Quarter FY 2019 = \$301,469
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$
- 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$
- 7. Projected carryover into FY 2020 = \$69,907 (8%)

#### MAJOR ACCOMPLISHMENTS

- 1. LLNL received 80 DVD copies of the 2017 edition of the ICSBEP Handbook on January 7, 2019 and promptly distributed 75 to preregistered NCSP users. An additional 80 DVDs are scheduled for receipt early next quarter (IPD1).
- 2. All NCSP evaluations were approved pending adequate resolution of the TRG comments at the ICSBEP meeting (IPD1) on October 22, 2018 including:
  - IER-407, FUND-LLNL-ALPHAN-U235-MULT-001, ISSA Subcritical Multiplicity Benchmark, LLNL
  - IER-422, FUND-NCERC-PU-HE3-MULT-003, Copper and Polyethylene-Reflected Plutonium Metal Sphere Subcritical Measurements (SCRaP), LANL
  - IER-451, LEU-COMP-THERM-099, Titanium and Aluminum Sleeve Experiments in Fully-Reflected Water-Moderated U(4.31)O<sub>2</sub> Fuel Rod Lattices with 2.8 cm Pitch, SNL
- 3. Providing NCSP website updates as requested by NCSP Management (IPD2).
- 4. Completed preliminary design of a prototype NDA website at <a href="https://nda-dev.llnl.gov">https://nda-dev.llnl.gov</a>, and submitted it to LLNL Information Management for review and release. The public version will be available early next quarter at <a href="https://nda.llnl.gov">https://nda.llnl.gov</a> (IPD2).
- 5. Performed required updates to NTS-SLAN/NCERC classified network images and servers to ensure the latest Microsoft patches were installed as required and performed required monthly "authenticated" scans for NCERC network devices. Provided hardware inventory per data call from LANL ISSM. Started annual self-assessment on NTS-SLAN as required for continuous monitoring and accreditation (IPD2).
- 6. Provided equipment inspections, certifications and data transfers (IPD2) in support of:
  - IER-184: TEX (LLNL)
  - IER-465: Non-NCSP NDSE Experiments in FY16 and FY17 (LANL)
  - IER-466: LANL IE1 NCERC Operational Support at the DAF (LANL)
  - IER-503: Non-NCSP Crit Class for JTOT (LANL)
- "Hot Box" laboratory reports, memoranda, drawings, etc., were compiled and reviewed this period as the first step in selecting a specific set of experiments for ICSBEP evaluation (IPD4).

#### **LLNL IP&D Milestones:**

Complete	On Schedule	Behind Schedule Missed Milesto		

QUARTER	MILESTONE	STATUS	COMMENTS
Q1	Manage all aspects of the DOE NCSP participation in the ICSBEP as required to		First 75 DVD copies of 2017 edition of the Handbook
	ensure the finalizing and publishing ICSBEP evaluations per IE schedule. (IPD1)		distributed to NCSP users.
	Provide status reports on LLNL participation in US and International IPD		All NCSP evaluations presented at the 2018 ICSBEP TRG
	collaborations (including ICSBEP) and provide brief summary report to NCSP		Meeting are approved pending resolution of the review
	Manager on items of NCSP interest. (IPD1)		comments.
	Maintain, operate and modernize he NCSP website, databases, and provide user		https://nda.llnl.gov_deployed.
	assistance as required. (IPD2)		
	Provide a status report for the evaluation of the LLNL "Hot Box" for inclusion in		Data collection completed this quarter. Evaluation to
	the ICSBEP Handbook. (IPD4)		commence next quarter.
Q2	Manage all aspects of the DOE NCSP participation in the ICSBEP as required to		
	ensure the finalizing and publishing ICSBEP evaluations per IE schedule. (IPD1)		
	Provide status reports on LLNL participation in US and International IPD		
	collaborations (including ICSBEP) and provide brief summary report to NCSP		
	Manager on items of NCSP interest. (IPD1)		
	Maintain, operate and modernize he NCSP website, databases, and provide user		
	assistance as required. (IPD2)		
	Provide a status report for the evaluation of the LLNL "Hot Box" for inclusion in		
	the ICSBEP Handbook. (IPD4)		
Q3	Manage all aspects of the DOE NCSP participation in the ICSBEP as required to		
	ensure the finalizing and publishing ICSBEP evaluations per IE schedule. (IPD1)		
	Provide status reports on LLNL participation in US and International IPD		
	collaborations (including ICSBEP) and provide brief summary report to NCSP		
	Manager on items of NCSP interest. (IPD1)		
	Maintain, operate and modernize he NCSP website, databases, and provide user		
	assistance as required. (IPD2)		
	Provide a status report for the evaluation of the LLNL "Hot Box" for inclusion in		
	the ICSBEP Handbook. (IPD4)		

Q4	Manage all aspects of the DOE NCSP participation in the ICSBEP as required to	
	ensure the finalizing and publishing ICSBEP evaluations per IE schedule. (IPD1)	
	Provide status reports on LLNL participation in US and International IPD	
	collaborations (including ICSBEP) and provide brief summary report to NCSP	
	Manager on items of NCSP interest. (IPD1)	
	Maintain, operate and modernize he NCSP website, databases, and provide user	
	assistance as required. (IPD2)	
	Provide a status report for the evaluation of the LLNL "Hot Box" for inclusion in	
	the ICSBEP Handbook. (IPD4)	

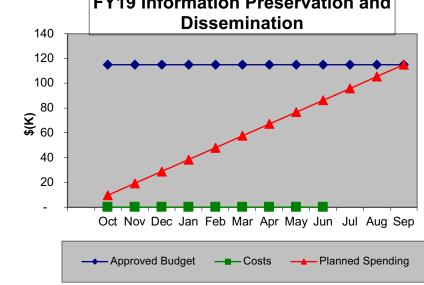
NCSP Element and Subtask: ORNL - IPD5, 6

**Task Titles:** 

IPD5-Oak Ridge Health Physics Research Reactor CAAS Benchmark Evaluation IPD6- Preservation and Dissemination of Unpublished Critical Experiments by Mihalczo

**M&O Contractor Name:** ORNL **Point of Contact Name:** Doug Bowen **Point of Contact Phone:** (865) 576-0315





- 1. Carryover into FY 2019 = \$0K
- 2. Approved FY 2019 Budget = \$115K (includes carryover)
- 3. Actual spending for 1<sup>st</sup> Quarter FY 2019 = \$0K
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$
- 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$
- 7. Projected carryover into FY 2020 = \$

MAJOR ACCOMPLISHMENTS

Reference: DP0909010/ORNL

Date of Report: January 20, 2019

#### IPD5 – Oak Ridge Health Physics Research Reactor CAAS Benchmark Evaluation

- This project is being led by Richard Hale at ORNL. He has created a team to review documents to be found as part of the literature search effort to find relevant documents that could be useful to generate CAAS benchmark reports
- Initiated a review documents in ORNL document records to identify potential HPRR/DOSAR reports of interest.
- The spending plot at left is not correct; work has started and the spend rate will increase.

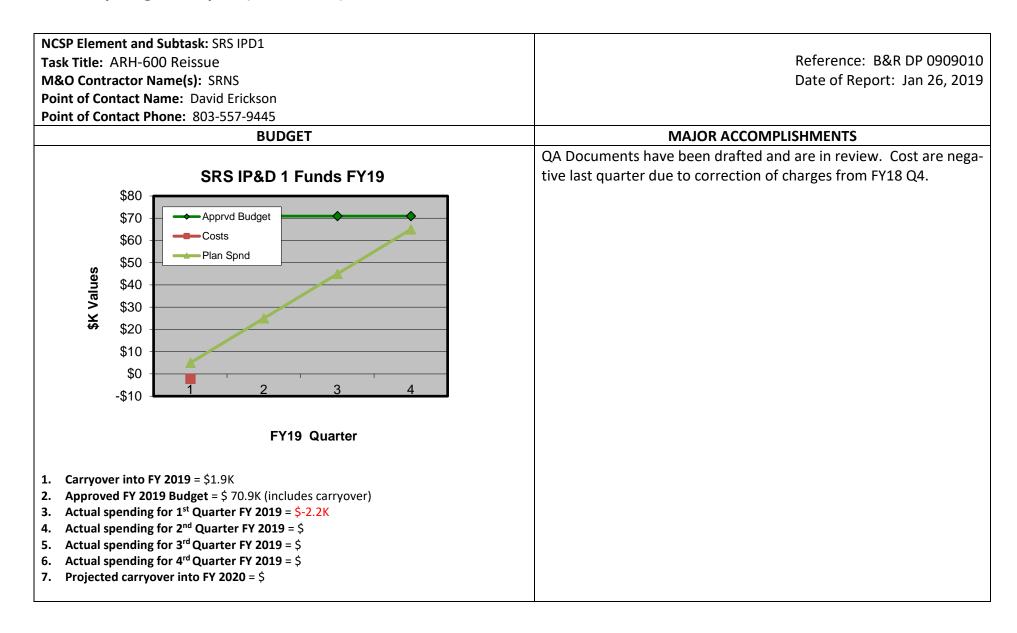
# IPD6 – Preservation and Dissemination of Unpublished Critical Experiments by Mihalczo

- A kickoff meeting was held in October 2018 with John Mihalczo, B.J. Marshall, Doug Bowen, and Justin Clarity. This was a Thomas Miller-led task. Progress is slow due to the lack of resources at this stage.
- A list of benchmark experiments was reviewed
- John provided logbook data; however, the data needs to be extracted from legacy tapes. An ORNL POC will be contacted in Q2 to extract the data for the list of proposed experiments provided by John.
- A subcontractor will likely be engaged on this project to determine if complete benchmark data exists to propose additional work in the outyears.

## **ORNL IPD Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

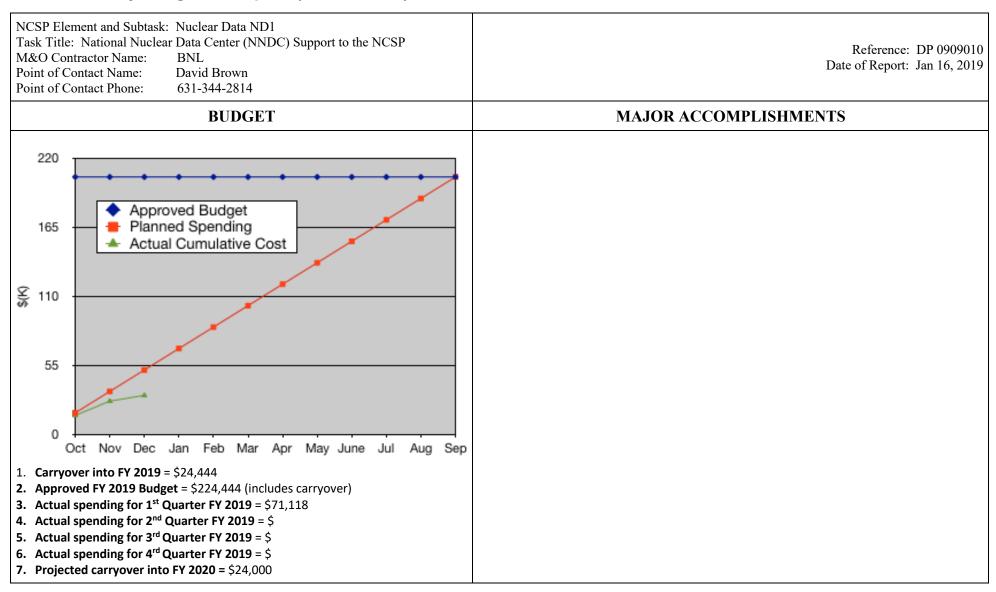
QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	NONE		
Q2	Complete documentation of data needed for an ICSBEP benchmark based on the ORNL HPRR (IPD5)		
Q3	Perform initial evaluation of HPRR data and determine if this task should continue (IPD5)		
Q4	Perform some initial benchmark simulations to evaluate the quality of the data collect in IPD5 and the ability to simulate the measured data (IPD5)		
	Report on progress made with the review of 25 critical experiments and their potential applicability and quality for generating ICSBEP evaluations in an FY20 NCSP proposal (IPD6)		



## SRS IP&D Milestones:

Ī	Complete	On Schedule	Behind Schedule	Missed Milestone
	Complete	On schedule	Berlind Schedule	Wiissed Willestone

QUARTER	MILESTONE	STATUS	COMMENTS
Q1	Provide status reports on SRS progress. (IPD1)		
Q2	Provide status reports on SRS progress. (IPD1) Develop QA documents for current version to meet current SRS/DOE requirements. (IPD1)		
Q3	Provide status reports on SRS progress. (IPD1)		
Q4	Provide status reports on SRS progress. (IPD1)		
	Issue Preliminary (updated) CritView version for internal testing. (IPD1)		
	Issue Preliminary User Guide to support internal testing. (IPD1)		



## **BNL ND Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Maintain and upgrade ADVANCE code system by performing data verification of new NCSP evaluations and performing quality assurance on the data as required and provide status reports on all nuclear data support activities to the NCSP Manager. (ND1)		Porting ADVANCE (and all of its dependencies) to Python3 is taking longer than anticipated. Also, actively interviewing for potential NCSP post-doc.
Q2	Maintain and upgrade ADVANCE code system by performing data verification of new NCSP evaluations and performing quality assurance on the data as required and provide status reports on all nuclear data support activities to the NCSP Manager. (ND1)		
Q3	Maintain and upgrade ADVANCE code system by performing data verification of new NCSP evaluations and performing quality assurance on the data as required and provide status reports on all nuclear data support activities to the NCSP Manager. (ND1)  If mandated by CSEWG, release new ENDF library. (ND1)		
Q4	Maintain and upgrade ADVANCE code system by performing data verification of new NCSP evaluations and performing quality assurance on the data as required and provide status reports on all nuclear data support activities to the NCSP Manager. (ND1)		

NCSP Element and Subtask: LANL ND1

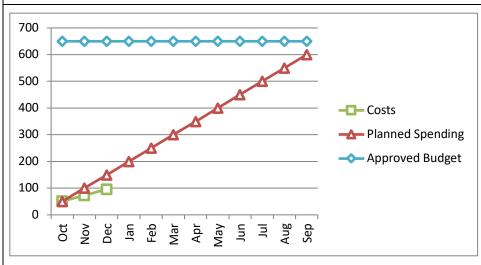
Task Title: Nuclear Data Evaluation and Testing

M&O Contractor Name: LANL

Point of Contact Name: Bob Margevicius / Bob Little Point of Contact Phone: 505-665-8965 / 505-665-3487

Reference: DP0909010 Date of Report: January 25, 2019

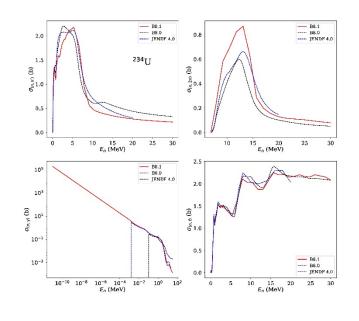
#### BUDGET



- 1. Carryover into FY 2019 = \$0
- 2. Approved FY 2019 Budget = \$650,000 (includes carryover)
- 3. Actual spending for  $1^{st}$  Quarter FY 2019 = \$96,044
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for  $3^{rd}$  Quarter FY 2019 = \$
- 6. Actual spending for  $4^{rd}$  Quarter FY 2019 = \$
- 7. Projected carryover into FY 2020 = \$50,000

#### MAJOR ACCOMPLISHMENTS

• 234U: reevaluated the fission cross section to include data by Tovesson et. al. The capture data taken at LANSCE has not been analyzed, so it cannot be directly used in the evaluation. However, the parameters of CoH3, used in the evaluation, have been adjusted to reproduce the LANSCE data for capture on 238U and 236U. A working ENDF file has been produced and tested successfully using the ENDF checking codes. The new evaluation differs significantly from the current version released (see current comparisons below showing current work (B8.1) compared to ENDF/B-VIII.0 and JENDF 4.0).



NCSP Quarterly Progress Report (FY-2019 Q1)	
	<ul> <li>236U: reevaluated the fission cross section to include data by Tovesson et. al. The resonance parameters for capture, determined from the measurements at LANSCE, have been put into ENDF-6 format, and are in the testing stages.</li> <li>Los Alamos scientists chaired two sessions at the November CSEWG meeting – the Evaluations and Covariance sessions.</li> <li>Los Alamos scientists gave 11 presentations at the November CSEWG meeting on topics including evaluation and theory work, validation studies, covariance updates, processing, measurements, and international collaborations.</li> <li>Los Alamos scientists are strong contributors to International activities such as the NEA SG-43 working to define an interface to GNDS, and the IAEA coordinated standards effort (updates to Pu239 fission cross section and PFNS).</li> </ul>

## **LANL ND Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports on LANL participation in US and International Nuclear Data collaborations. (ND1)		
	Conduct CSEWG Data Evaluation Committee session. (ND1)		
	Report data testing results with ENDF/B-VIII.0 and additional beta release cross sections. (ND1)		
Q2	Provide status reports on LANL participation in US and International Nuclear Data collaborations. (ND1)		
Q3	Provide status reports on LANL participation in US and International Nuclear Data collaborations. (ND1)		
Q4	Provide status reports on LANL participation in US and International Nuclear Data collaborations. (ND1)		
	Report on development of machine learning tools, in particular decision trees, for criticality-safety applications and sensitivity to nuclear data. (ND1)		
	Deliver nuclear data evaluations as indicated in Appendix B of this document. (ND1)		

NCSP Element and Subtask: ND1, 2, 3, 5, 6

Task Titles: See last page for full task titles

ND1 Delayed fission gammas

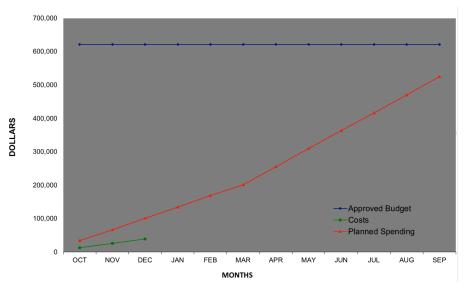
ND2 Generation and testing of thermal scattering laws

ND3 FLASSH (modern code)
 ND5 Advanced Doppler Broadening
 ND6 Cadmium radiative capture gammas

**M&O Contractor Name:** Lawrence Livermore National Laboratory

**Point of Contact Name:** David Heinrichs **Point of Contact Phone:** (925) 424-5679





- Carryover into FY 2019 = \$181,360
- Approved FY 2019 Budget = \$621,360 (includes carryover)
- 3. Actual spending for 1st Quarter FY 2019 = \$39.066
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$
- 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$
- 7. Projected carryover into FY 2020 = \$96,360 (15%)

Reference: B&R DP0909010

Date of Report: January 25, 2019

#### MAJOR ACCOMPLISHMENTS

- 1. The feasibility of extending LLNL's delayed fission gamma methodology to beta particle emission (for subsequent bremsstrahlung gamma production) is being assessed. (ND1)
- 2. NCSU examined and modified the diffusional model parameters used in calculating the TSL for light water. In particular, the model is now consistent in extracting its input (for LEAPR calculations) from a combination of the performed MD simulations and the analysis of Novikov et al (Journal of Structural Chemistry, Vol. 31, No.1, pp. 77-85, 1990). Testing was performed to verify the sensitivity of the TSL to various MD model and diffusional model parameters and it was found that the TSL is most sensitive to the value of the O-H bond length that is used in the MD analysis. Using the finalized parameters, the TSL libraries were generated in the temperature range 283 to 623 °K. The TSL package will be transmitted upon finalizing QA checks. In addition, the approach for MD/DFT modeling for hydrofluoric acid and uranium hexafluoride (HF+UF6) was explored during this period. The focus has been on identifying various operational conditions for these materials and the appropriate simulation methods under these conditions. In addition, the properties of this HF+UF6 eutectic was collected including the phase diagram and other fundamental properties such as density and diffusivity. (ND2)
- 3. NCSU continued work on the FLASSH code. The addition of a module for the treatment of liquids in FLASSH has been initiated. The module reads in the alpha/beta grid and the solid  $S(\alpha,\beta)$  from the FLASSH output, while also reading in the diffusive input parameters from the user. Using these inputs, the module calls the 'convolution\_grid' algorithm to interpolate the TSL onto a fine grid for properly convoluting the complete shape of the diffusive peak (this diffusive peak goes with a corresponding diffusive model, e.g., Langevin). Inside this 'convolution\_grid' algorithm, a function is called to evaluate the liquid model, and the 'interp\_grid' algorithm is called to move from one grid resolution to another as needed. Finally, the 'convolve' algorithm is called to perform the convolution, add in the Debye-Waller term, and to construct the total  $S(\alpha,\beta)$ . The results are then output to a file. Implementation of this module into the FLASSH code also includes adding new input in the FLASSH input file, making use of global shared variables already present in FLASSH during evaluation (e.g. nalpha, nbeta, etc.), adding other liquid models, and outputting

results to <i>FLASSH</i> output. In addition, the algorithm for calculating the angular distribution for particle scattering in equal probability bins has advanced this period. The programing into <i>FLASSH</i> is proceeding and initial testing has started. Under the current ACE library, the angular portion of the double differential cross section is tabulated as equal probability angular bins. At each specific neutron incident energy, the scattering probability is the same within each bin. These bins are evaluated by a progressive bin search algorithm. This algorithm might result in unexpected extrapolation result. Alternatively, <i>FLASSH</i> adapts an interpolation-based search algorithm to find the equal probable angular bins. The algorithm is currently under testing. (ND3)
<ul> <li>4. NCSU continued the development of algorithms using a generalized non-cubic treatment in the calculation of the TSL. In <i>FLASSH</i>, the implementation of the non-cubic treatment takes into account the Debye-Waller matrix and the reciprocal space polarization information. Direct sampling of reciprocal space is used in the algorithm and replaces the use of the phonon density of states as performed in the current treatment (e.g., LEAPR/NJOY). In the phonon expansion, the density of states is no longer used in the convolution. Alternatively, a grid with 8000 reciprocal space points per Brillouin zone is applied in the evaluation of the dynamic structure factor across the whole reciprocal space. Subsequently, the evaluated structure factor is interpolated to a much finer grid. The S(α,β) is evaluated by binning the four-dimensional structure factor to the α shells and β bins. The finer grid would increase the quality of statistics in the evaluation of S(α,β) in the binning process. The developed algorithm is implemented as a new module in <i>FLASSH</i>. The non-cubic module supplies the α and β grid from the input module and reads from a standalone input file the polarization vector at 8000 reciprocal space points. The evaluation and interpolation algorithm are the same as used in the one phonon correction module. The developed module can be executed in parallel with any available number of computational threads via OpenMP binding. (ND5)</li> <li>5. Planning in progress for an improved measurement of radiative capture gammas using a thermal beam line at the UC-Davis McClellan reactor. (ND6)</li> </ul>

#### **LLNL ND Milestones:**

STATUS (copy color code and paste below in 'STATUS' field)

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	COMMENTS
Q1	Provide status on LLNL/NCSU nuclear data activities to NCSP Manager (ND1 {subtask 1 and 2}, ND2, ND3, ND5, ND6).		
Q2	Provide status on LLNL/NCSU nuclear data activities to NCSP Manager (ND1 {subtask 1 and 2}, ND2, ND3, ND5, ND6).		
Q3	Provide status on LLNL/NCSU nuclear data activities to NCSP Manager (ND1 {subtask 1 and 2}, ND2, ND3, ND5, ND6).		
Q4	Provide status on LLNL/NCSU nuclear data activities to NCSP Manager (ND1 {subtask 1 and 2}, ND2, ND3, ND5, ND6).		
	Deliver thermal neutron scattering data evaluations as indicated in Appendix B of the 5-Year Plan. (ND2)		Evaluations completed one or more years in advance of schedule.

#### **Task Titles:**

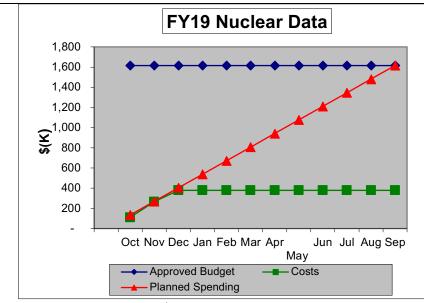
- ND1 Subtask 1 Delayed Fission Gamma Multiplicity and Spectra Data testing
- ND1 Subtask 2 Delayed Fission Gamma Multiplicity and Spectra Document the technical basis of the method and data testing results
- ND2 Generation and Benchmarking of Thermal Neutron Scattering Cross Sections in Support of Advanced Nuclear Reactor Concepts
- ND3 Development and Implementation of an Advanced and Rigorous Computational Platform for Thermal Neutron Scattering Analysis
- ND5 Development and Implementation of a Modern Doppler Broadening Approach Including Atomic Binding Effects
- ND6 Evaluate Neutron Radiative Capture Gamma Production in Cadmium

NCSP Element and Subtask: ORNL – ND1, 3, 6, 7, 10 Task Title: see last page

M&O Contractor Name: ORNL
Point of Contact Name: Doug Bowen
Point of Contact Phone: (865) 576-0315

Reference: DP0909010/ORNL Date of Report: January 20, 2019

#### **BUDGET**



- 1. Carryover into FY 2019 = \$124K
- 2. Approved FY 2019 Budget = \$1,615K (includes carryover)
- 3. Actual spending for 1<sup>st</sup> Quarter FY 2019 = \$379K
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$
- 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019Y = \$
- 7. Projected carryover into FY 2020 = \$

#### **MAJOR ACCOMPLISHMENTS**

#### ND1 - Evaluations and Measurements

- Status report on all nuclear data support activities.
  - Participated in the CSEWG meeting in November 2018 at BNL and gave a presentation about NCSP cross section experimental activities for La.
  - Worked on action sheet 66 for the DOE-Euratom agreement under which the future JRC-ORNL experiments for the NCSP will be performed at the JRC-Geel.
  - Support of post-doc for Ce data analysis.
  - Work on updating Appendix B for the NCSP five-year plan.
  - Supporting cerium evaluations (on schedule)
  - Analysis on the experimental database was discussed for both cerium isotopes 140,142Ce
  - Inconsistencies such as aluminum impurities and sample thickness in the experimental database were discussed and, in some instances, clarified
  - Work on the draft of the ORNL/TM report was performed
  - Review of the abstract for ICNC2019
  - Preliminary work on 233U (on schedule)
  - Work on determining the average deviation between ORELA and nTOF fission data
  - Initial fit of the fission cross section to the nTOF data
  - Silicon evaluation: evaluation and validation (completed)
  - o Inclusion of an improved direct capture cross section component
  - Generation of the ENDF files and submission for validation
  - Work on the letter report
  - Work on the presentation for Nuclear Data Week 2018
  - Attendance to the Nuclear Data Week at BNL in November 2018.
  - Gd-156,158,160 (On Schedule)
    - Resolved resonance region evaluation of differential experimental nearing completion. In Business Quarter 1 of Fiscal Year 2019, resolved resonance region parameters for Gd-156,158,160 evaluated at ORNL were synchronized with the resolved resonance parameters for Gd-155,157 being concurrently evaluated at IRSN. The two collaborators are preparing to make preliminary joint evaluation release for testing to the nuclear data community.

NCSP Element and Subtask: ORNL – ND1, 3, 6, 7, 10 Task Title: see last page M&O Contractor Name: ORNL Point of Contact Name: Doug Bowen Point of Contact Phone: (865) 576-0315	Reference: DP0909010/ORNL Date of Report: January 20, 2019
BUDGET	MAJOR ACCOMPLISHMENTS
BUDGET	Pb-204,206,207,208 (On Schedule) Initial fitting of differential experimental data has begun for the isotopes of lead. Particular attention is given to the identification of the quantum angular momentum group structure for the resonances of Pb-207 which where previously incorrect due to outdated ENDF format restrictions.  Foreign Travel (Foreign travel report delivered to NCSP manager) IAEA for International Nuclear Data Evaluation Network (INDEN) meeting on structural materials. Sobes attended representing resonance evaluation capabilities of ORNL. Details are provided in the foreign travel report  National Collaboration Sobes attended the US National Nuclear Data Week at the National Nuclear Data Center to discuss the future of nuclear data evaluations beyond ENDF/B-VIII.0  Complete cross-section measurement and evaluation deliverables per the nuclear data schedule in Appendix B of the 5-year plan.  Travel to JRC-Geel to initiate Ce-142 experiments (green) Travel to JRC-Geel to performed data reduction for La capture experiments. The list mode data were sorted into TOF spectra. (green) Finalized reduction for the thick La sample transmission experiments. Transmission factors for La obtained. (blue) La transmission data was tested for analysis with SAMMY. Obtained additional information for planned Cl(n,p) experiments from previous experiments performed at JRC. Path forward: continue data sorting for La capture data. Start in 2019 Ce-142 experiments. Enriched Zr experiments are delayed, due to problems obtaining samples for lease. (behind schedule). However, this issue seems to be resolved. Path forward: After finalizing the Ce-142 experiments, enriched Zr neutron capture experiments will be started.
	<ul> <li>Y12 ND1 – GELINA depleted Uranium target cost estimate and construction</li> <li>During the last travel to JRC, drawings were brought to JRC and checked by JRC personnel. Organized and participated in telecon between JRC and Y12 personnel concerning final target drawing. All outstanding issues were resolved.</li> </ul>

NCSP Element and Subtask: ORNL – ND1, 3, 6, 7, 10 Task Title: see last page M&O Contractor Name: ORNL Point of Contact Name: Doug Bowen Point of Contact Phone: (865) 576-0315	Reference: DP0909010/ORNL Date of Report: January 20, 2019
BUDGET	MAJOR ACCOMPLISHMENTS
	<ul> <li>ND3 – Isotopic Sample Lease to Support ND1 ND Measurements</li> <li>Ce-142 sample was leased in early fall from ORNL for neutron induced cross section experiments at JRC. (green)</li> <li>Sample shipped to JRC. However, due to problem in enclosing the samples in the Al can, the sample did not arrive in timely manner to start experiments during the last travel. Also, the shipped Al can for the empty sample had to be redone due to bad welding. (green / behind schedule)</li> <li>Pre Q1FY2019 activities: Performed activation experiments on Ce142 with a result of no activity detected. Performed SCALE and ORIGEN calculation for the enriched Ce-142 samples including all minor isotopes and impurities of the sample. In addition, (γ,n) activation calculation were performed since the electron accelerator driven neutron sources are also intense gamma- ray sources. (green)</li> </ul>
	<ul> <li>ND6 - Sammy Modernization</li> <li>Prepared the FY2018 ND6 deliverable: "FY2018 Nuclear Criticality Safety Program, ORNL Nuclear Data Subtask 6 (ND6): SAMMY Modernization" Sponsor Report, ORNL/SPR-2018/1075 (2018).</li> <li>Prepared and presented a presentation titled "SAMMY Modernization and Advances in Nuclear Data Evaluation Methods" at the annual nuclear data community meeting at the Cross Section Evaluation Working Group Meeting at the Brookhaven National Laboratory, Nuclear Data Week, November 5-9, 2018. This is to inform Nuclear Data community of the SAMMY Modernization progress.</li> <li>Prepared an abstract titled "Modernization of SAMMY: An R-matrix Bayesian Nuclear Data Evaluation Code" for the 2019 International Conference on Nuclear Data for Science and Technology, May 19-24, 2019, Beijing, China. The abstract has been accepted for an oral presentation at this major international nuclear data conference.</li> <li>Leveraged ENDF C++ interfaces originally developed for AMPX by incorporating these interfaces into SAMMY. This will ensure that modernized SAMMY will be able to read the latest ENDF format and will minimize code maintenance by code sharing with AMPX and SCALE, that is a long term strategy for modernized SAMMY.</li> </ul>

NCSP Element and Subtask: ORNL – ND1, 3, 6, 7, 10	Reference: DP0909010/ORNL
Task Title: see last page	Date of Report: January 20, 2019
M&O Contractor Name: ORNL	
Point of Contact Name: Doug Bowen	
Point of Contact Phone: (865) 576-0315	
BUDGET	MAJOR ACCOMPLISHMENTS
	<ul> <li>Implemented Brune transformation between the formal R-matrix parameters and the alternative R-matrix parameters derived by Carl Brune in Physical Review C66, 044611, https://doi.org/10.1103/PhysRevC.66.044611.  Brune transformation will enable evaluators to verify resonance energies that, thanks to the Brune transform, can be unambiguously identified with peaks in the measured cross sections.</li> <li>Several SAMMY bug fixes and optimizations.</li> </ul>
	ND7 - Nuclear Data Evaluation and Testing for Nuclear Criticality Safety Applications    This work is being done by Alex Shaw at Ga Tech for MS degree.
	The student took S/U training at ORNL during the fall training block. After the training, the student has started to familiarize himself with MCNP, KENO, the ICSBEP handbook, and DICE. The student began the arduous process of using DICE to find and select benchmarks that will be most strongly impacted by the isotopic and thermal moderator changes in ENDF-VIII.0 (specifically, isotopes and thermal moderators listed in Appendix B-1 and B-2, respectively, of the most recent edition of the NCSP five-year plan). Student has been mentored on the importance of appropriate benchmark selection and the impact of the nuclear data on the benchmark calculations. The student is on track to finalize the selection of relevant ICSBEP experiments in Q2.
	ND10 - Monte Carlo Evaluation of Differential and Integral Data
	<ul> <li>Assembled the ORNL team members and defined their roles in this project.</li> <li>Submitted an application for 70 million CPU hours to the Director's Discretionary fund at the Oak Ridge Leadership Computing Facility (OLCF: olcf.ornl.gov).</li> <li>Derived mathematical equations to be programmed on the OLCF supercomputers.</li> <li>2 months late in initiating work because funding was allocated in late November.</li> </ul>

# **ORNL ND Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports (ND1, ND3, ND6, ND7, ND10).		
	Provide status reports on ORNL participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest (ND1).		
	Complete cross-section measurement and evaluation deliverables per the nuclear data schedule in Appendix B (ND1).		Behind schedule with Ce-142 measurements due to sample shipping delays and a bad Ce-142 Al can weld that had to be redone.
Q2	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports (ND1, ND3, ND6, ND7, ND10).		
	Provide status reports on ORNL participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest (ND1).		
	Complete cross-section measurement and evaluation deliverables per the nuclear data schedule in Appendix B (ND1).		
Q3	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports (ND1, ND3, ND6, ND7, ND10).		
	Provide status reports on ORNL participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest (ND1).		
	Complete cross-section measurement and evaluation deliverables per the nuclear data schedule in Appendix B (ND1).		
Q4	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports (ND1, ND3, ND6, ND7, ND10).		

Provide status reports on ORNL participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest (ND1).	
Complete cross-section measurement and evaluation deliverables per the nuclear data schedule in Appendix B (ND1).	
Document SAMMY modernization progress and report status annually to the NCSP Manager (ND6).	

#### **Task Titles:**

ND1 Nuclear Data Measurement and Evaluation

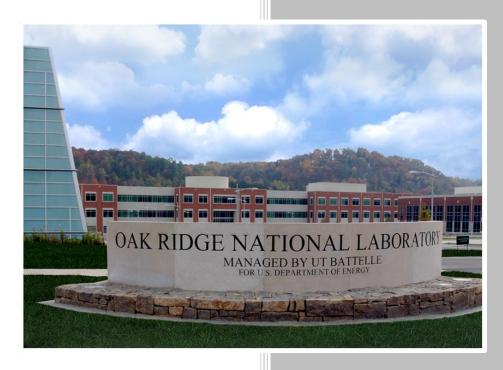
ND3 Isotopic Sample Leases to Support ND1 ND Measurements

ND6 SAMMY Nuclear Data Evaluation Code Modernization

ND7 Nuclear Data Evaluation and Testing for Nuclear Criticality Safety Applications

ND10 Monte Carlo Evaluation of Differential and Integral Data

# FY2018 Nuclear Criticality Safety Program, ORNL Nuclear Data Subtask 6 (ND6): SAMMY Modernization



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December 2018

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#### ORNL/SPR-2018/1075

Reactor and Nuclear Systems Division

## FY2018 Nuclear Criticality Safety Program NUCLEAR DATA SUBTASK 6 (ND6): SAMMY MODERNIZATION

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Date Published: December 2018

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UT-BATTELLE, LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

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#### 1. EXECUTIVE SUMMARY

This modernization effort was undertaken to make incremental improvements to the SAMMY Fortran legacy code. These improvements are vital to ongoing nuclear data evaluations at Oak Ridge National Laboratory, and they also serve to sequentially modernize parts of the SAMMY code. This effort involves a two-pronged approach to SAMMY modernization. High-priority new features recently requested by the nuclear data evaluation community would be implemented into the SAMMY code. The SAMMY source code would also simultaneously undergo a sequential modernization of its modules. This will ensure that the most current SAMMY version will contain the newest features and the latest updates.

Ideally, modernization of a given legacy SAMMY module should implement new features that in most cases would not have been possible prior to the modernization. Such synergy between module modernization and new feature implementation was achieved during FY2018 with the introduction of a modernized C++ implementation of Coulomb functions. This update was essential for computing the effects of previously neglected closed channels used in the computation of nuclear cross sections in nuclear data evaluations. Indeed, the effects of closed channels could not have been computed by the legacy implementation of Coulomb functions.

In addition to modernizing SAMMY Coulomb functions and implementing essential new features, other new features have been implemented as requested by nuclear data evaluators. Furthermore, other aspects of the legacy Fortran SAMMY code modernization, such as replacing deprecated Fortran COMMON blocks with Fortran 90 modules, were achieved in FY2018.

During FY2018, the following *new features* have been implemented:

- 1. The effect of closed channels previously ignored in the legacy version of SAMMY, has been included for more accurate computation of cross sections that conforms to *R*-matrix formalism.
- 2. The effect of closed channels has also been included in the computation of analytical *derivatives* of cross sections, which are used in SAMMY for updating *R*-matrix resonance parameters during evaluation of *R*-matrix resonance parameters for ENDF.
- 3. Brune's transformation between *formal R*-matrix parameters and *physical R*-matrix parameters has been implemented to enable intuitive identification and tracking of resonances in the process of nuclear cross-section evaluation using the SAMMY code.

The features listed above were made possible by the following module modernization efforts completed during FY2018:

- 1. Modernization of Coulomb functions was introduced to SAMMY to enable implementation of features 1–3 listed above.
- 2. Fortran 77 legacy COMMON blocks were replaced by Fortran 90 modules.
- 3. A list of features slated for the SAMMY 8.2 release scheduled for FY2019 has been finalized and mostly implemented during FY2018.
- 4. Preparations for the open source release of SAMMY 8.2 are well under way and conform with Oak Ridge National Laboratory (ORNL) procedures for releasing open source codes.

The new features listed above have been implemented within the SAMMY application programing interface (API) and the software quality assurance (SQA) framework outlined in the FY2017 SAMMY Modernization Report [1].

#### 2. SAMMY BACKGROUND INFORMATION

SAMMY [2] is an ORNL-developed legacy code used worldwide to evaluate nuclear differential reactions cross-section data in resolved and unresolved resonance energy ranges induced by incoming neutrons, protons, and  $\alpha$ -particles. SAMMY updates prior values of phenomenological nonrelativistic R-matrix resonance parameters via the Newton-Raphson iterative minimization of generalized  $\chi^2$ -function to yield optimal posterior resonance parameter values, their covariance matrix, and the corresponding evaluated nuclear data and covariance matrix [3]. SAMMY accounts for various experimental effects that are custom-tailored to several leading measurement facilities and detectors. Over several decades, SAMMY has become an important tool for nuclear data resonance parameter evaluations disseminated via ENDF for simulations of nuclear systems by neutron transport code systems such as SCALE [4] and MCNP [5].

To implement a modernization project of the magnitude required, and in view of SAMMY's vast feature set implemented entirely in old-fashioned serial FORTRAN 77, the overarching goals of the SAMMY modernization project are to improve maintainability, modularity, feature extensibility, and computer performance by using modern, object-oriented development, quality assurance, and high-performance computing frameworks. This goal was pursued in the coordinated tasks and activities described below to ensure a smooth transition from the legacy SAMMY code to a completely modernized SAMMY version.

- 1. In FY2017, SAMMY 8.0.0 was ported into a modern SQA framework by modernizing and automating its build and test system. This was accomplished by leveraging the SQA system already adopted by ORNL's SCALE [4] and AMPX [6] code systems. The SAMMY 8.1.0 release was completed and made available to the public via ORNL's Radiation Safety Information Computational Center (RSICC) in April 2017.
- 2. The SQA platform established in step 1 was used as the foundation for making incremental changes to the legacy SAMMY code while supporting ongoing nuclear data evaluations at ORNL and elsewhere. When possible, API-based programming was used to enable comparisons between the results of the legacy system and the modernized implementations of an API to divide SAMMY modernization into tractable tasks.
- 3. In parallel with step 2, design and implement various APIs for C++ modernized SAMMY modules to be developed entirely within this modern SQA framework, thus enabling source code sharing with SCALE and AMPX code systems, which already employ the API programming model.
- 4. Generalize and modernize mathematical and physical methods implemented in the legacy SAMMY 8.0.0 code, and implement them strategically during modernization.
- 5. Anticipate future features and applications of modernized SAMMY to ensure that they will fit into the software framework of modernized SAMMY.

The FY2017 NCSP SAMMY Modernization Report [1] concluded that, as with SCALE and AMPX, the modernized SAMMY code should be written in C++ API framework using third-party high-performance libraries when optimal.

This framework will make it much easier to implement useful new SAMMY features and would enable SAMMY code to be shared seamlessly inside the SCALE and AMPX API-based framework.

#### 3. PIECEMEAL SAMMY MODERNIZATION

To enable modernization of individual SAMMY modules so that nuclear data evaluators can use the latest release of the SAMMY code while it is undergoing sequential modernization of its modules, the initial effort to completely modernize SAMMY in a single effort is no longer the objective. Instead, the *curiously recurring template pattern*<sup>1</sup> [7] shown in Figure 1 was adopted. Piecemeal modernization of a generic SAMMY module ("Module 1") is performed by:

- 1. Defining a C++ API for Module 1,
- 2. Implementing C++ API of Module 1 by:
  - a. Using the legacy Fortran code (by stripping it out of the legacy source code),
  - b. Using a modern or third-party C++ implementation,
- 3. Defining a variable in the C++ code whose value can be set by the user to use either implementation of Module 1 C++ API,
- 4. Testing for consistency between the two implementations using SAMMY test cases, and
- 5. Continuing forward with just the modernized implementation of Module 1 C++ API.



Fig. 1. A piecemeal modernization of Module 1 (e.g., Coulomb function module).

#### 4. CLOSED CHANNELS IN SAMMY

Since the legacy SAMMY code was originally conceived for nuclear data evaluations of resolved resonance ranges (RRRs) of heavy nuclides, with RRR generally confined to well below the threshold energy of their lowest endothermic<sup>2</sup> channel, effects of endothermic channels have been justifiably neglected. However, for RRR evaluations of low- and medium-mass nuclides such as oxygen or iron, where cross-section measurements typically span energies below and above endothermic channel thresholds, it has become necessary to account for the effect of endothermic channels not just *above* but also *below* their threshold energies to conform to exact *R*-matrix formalism.

The SAMMY subroutine responsible for computing the *R*-matrix cross sections has been modified significantly so that it exactly computes closed-channel contributions to resonance cross sections.

However, incorporating endothermic channels at energies below their thresholds, necessitates modernization of the SAMMY Coulomb function. This modernization was achieved by using a modern

<sup>&</sup>lt;sup>1</sup> For more information, please see https://en.wikipedia.org/wiki/Curiously recurring template pattern.

<sup>&</sup>lt;sup>2</sup> Endothermic channels become open at neutron energies larger than some *positive* channel threshold energy.

C++ library [8] to implement the new C++ Coulomb function API for the SAMMY code as described in Section 5.

The inclusion of closed channels was possible because of the new Coulomb wave function (CWF) API and the SAMMY modernization that was implemented in FY2018. Without these, SAMMY could not compute shift factors below the channel threshold, which is needed to include the effect of closed channels in the *R*-matrix formulation. Furthermore, these improvements reduced code complexity by eliminating the need for many IF-ELSE branches and consolidated charge-specific subroutine calls into general subroutines, where particle charge is used as an input parameter.

#### 5. MODERNIZATION OF COULOMB FUNCTIONS

Computation of the closed channels below threshold energies requires the *R*-matrix shift functions to be computed at negative energies for which a corresponding momentum wave number is purely imaginary. This in turn, necessitates computation of Coulomb functions for the same imaginary values of momentum wave number. Because the Coulomb functions used by the legacy code have not been designed for imaginary values of the momentum wave number, a new modern implementation of Coulomb function was introduced to achieve this.

Therefore, a recently developed, modern C++ library of Coulomb functions over the largest known domain of complex input parameters [8] has been integrated into the SAMMY code to replace the legacy Fortran implementation. The license agreement negotiated with the author of this modern Coulomb library [8] has made the library easily accessible for linking with any SCALE or AMPX module, and its source code can be legally distributed within any ORNL code.

Consequently, a software design decision was made to move the modern Coulomb library into a central repository of SCALE third-party libraries. This has required some upfront reorganization of the repository structure and reconfiguration of the build and test environments. However, modern Coulomb functions are now available for easy linking and distribution by any other SCALE code including AMPX. It is expected that code sharing between SAMMY and AMPX, of which the modern Coulomb library is just one example, will enable rapid adoption of new evaluation techniques and new ENDF formats into AMPX processed libraries.

In the context of SAMMY implementation of phenomenological *R*-matrix formalism, Coulomb functions can be viewed as a tool for computing the *R*-matrix shift function and the penetrability needed for computation of cross sections. Because computation of the shift and the penetrability functions require special approximations of various limits of input parameters, several implementations are needed to compute them in SAMMY to control numerically divergent calculations.

The SAMMY code and the legacy implementation of Coulomb functions used by SAMMY were historically designed for real-valued arguments only. On the other hand, modern implementations of Coulomb functions are designed for complex-valued (i.e., complex data type) arguments. Consequently, some adjustments were needed when interfacing SAMMY to a modern Coulomb functions library, especially because the modern Coulomb library was not designed with the ultimate goal of computing the *R*-matrix shift and penetrability functions. This problem was solved by introducing a layer of indirection between the real-valued interface of the SAMMY code to the complex-valued interface of the modern Coulomb function library. Overall, the SAMMY source code was made simpler and more clear by the adoption of the modern Coulomb functions library.

The modern Coulomb library into the SAMMY code was implemented via a software design pattern known as the *curiously recurring template pattern* [7], that in this case has been implemented in the following four steps:

- 1. Create a C++ Coulomb functions API that abstracts the features needed to compute the R-matrix shift and penetrability functions.
- 2. Extract the legacy SAMMY code that currently provides those features out of SAMMY, and use it to implement the C++ API above.
  - a. This requires two steps of indirection: one between the Fortran SAMMY and the C++ API, and another between the C++ API and the extracted legacy implementation.
  - b. SAMMY test cases were run to ensure identical results were obtained, as expected.
- 3. Implement the C++ API created in step 1 via the modern Coulomb function implementation.
- 4. Switch from the extracted legacy Fortran implementation of the C++ API in step 2 to the modern Coulomb function implementation in Step 3 and rerun the test cases.

For an especially difficult combination of input parameters—namely, the  $\eta$  parameter much greater than the  $\rho$  parameter—the implementation of the *R*-matrix shift and the penetrability function in the legacy code relies on an accurate analytical approximation that avoids numerical singularities experienced by the Coulomb function for the same input parameters. Consequently, the research team retained the same analytical approximation used by the legacy code for this particularly difficult known case only, and it has been converted to its equivalent C++ implementation in the process of SAMMY modernization in FY2018.

The C++ Coulomb functions API previously implemented in FY2018 quarter 2 was extended in quarter 3 to provide the required Coulomb wave function (CWF) solutions for neutral particles (in addition to charged particles). The CWF API is designed with a layered software architecture approach, so the top-level complexity of computing the CWFs in the SAMMY source code is greatly reduced, improving readability, and long-term maintainability is ensured. The underlying solution methods used by the CWF API were improved to take advantage of well-known recursion relations to further reduce the complexity and computational cost of solving for the CWFs. Furthermore, the CWF API now caches the wave function solutions to reduce the number of solves required when computing intimately related quantities such as penetrability, shift factor, and phase shift.

As expected, these changes to the *R*-matrix subroutine resulted in no change to results of test cases utilizing the boundary condition B=S(E). On the other hand, results of test cases utilizing constant boundary conditions were examined for correctness and rebaselined as necessary (see section 10 for more information).

#### 6. MODERNIZATION OF SAMMY LEGACY FORTRAN INFRASTRUCTURE

To address long-term maintainability, all Fortran 77 COMMON blocks and BLOCK DATA have been completely eliminated from the SAMMY source code. These global data structures were reworked into modern Fortran module containers, which is a necessary first step in creating manageable libraries. This refactoring will also untangle some interdependencies inherent in the code, as well as improve clarity by allowing for explicit inclusion of individual variables as needed.

To facilitate weaning from legacy Fortran IMPLICIT data-type declaration statements, which are ubiquitous throughout the SAMMY code, in late FY2018, the team researched third-party source code processing codes as candidates for automated conversion from IMPLICIT Fortran data-type declarations

to EXPLICIT data types. This initiative included (1) contacting developers of those codes to obtain evaluation copy of their codes, (2) installing and testing their codes as to the fitness of purpose, and (3) researching corresponding documentation to ascertain their suitability for this task. It is hoped that automating the conversion to the explicit data-type declaration with one of these third-party codes would likely save a considerable amount of time and funds in converting Fortran legacy sections of SAMMY into a more modern, maintainable, and stable Fortran code.

#### 7. SAMMY BUG FIXES

Based on user feedback, the SAMMY PAR file was changed to keep Reich-Moore fission channel widths at zero if they were zero-valued in the ENDF file (i.e., specifically taken from the LRF = 3 format). The SAMMY code assumed all channels stay open once open (i.e., in a spin group), so it wrote a default value of  $10^{-7}$  eV for channel widths that were previously open but not given a width in ENDF. This affects only the intermediate SAMMY PAR file-write for LRF = 3, and LRF = 1,2,7 is unaffected. This change has virtually no impact on the fitted cross sections but greatly improves consistency and clarity for the user.

### 8. SAMMY USER SUPPORT

Support has been provided to ORNL SAMMY users, as well as to users at Los Alamos National Laboratory and Rensselaer Polytechnic Institute (RPI). Bug reports received from all users have been logged into a tracking system, Fogbugz, and are tracked until resolved. Each bug solution leads to creation of a new SAMMY test case that reveals the same bug, according to the SAMMY SQA guidelines.

Several particularly complicated bugs were uncovered by evaluators in the legacy SAMMY code. Because several workarounds do exist, it was determined that debugging of the legacy code would divert too much time and too many resources from SAMMY modernization to warrant their immediate resolution. Long-term SAMMY modernization will address these problems by replacing the legacy Fortran code with a modular C++ code.

#### 9. IMPROVED MODELING OF RADIATIVE NEUTRON CAPTURE YIELDS

Changes were made in SAMMY to improve modeling of radiative neutron capture reactions observed in neutron time-of-flight experiments. This has been achieved by using DICEBOX and Monte Carlo N-particle transport code to model capture photons escaping the sample of interest and interacting in capture detectors. An expression for the correction to the neutron capture yield as a function of the total cross section only allows for this correction to be included in the Bayesian fitting process performed by SAMMY.

#### 10. SOFTWARE QUALITY ASSURANCE

Using the successful conversion of SAMMY 8.0.0 into the modern SQA framework used for SCALE and AMPX development and release control in FY2017, the research team has continued to utilize this investment by maintaining, updating, and creating new test cases, as needed by the SAMMY modernization effort. FY2018 work involved using a versatile, multiplatform configuration (*cmake*) and testing (*ctest*) utilities, as has been described in the FY2017 NCSP SAMMY Modernization Report [1].

Key components of the SAMMY SQA include:

- Source code version control system (Mercurial, to be replaced by git)
- Automated build system for various platforms (*cmake*)
- Automated test system with user specified precision (*ctest*)
- Case management and bug tracking (Fogbugz, to be migrated to git)

The automated build and testing of the legacy code was enabled by the following combinations of Fortran compilers and operating systems: (1) GNU gfortran (versions 4 and 5), Linux, Mac OSX; and (2) Intel ifort FORTRAN compiler and Windows.

The SAMMY code SQA is built on nearly 190 composite test cases, some of which may have as many as two dozen subcases. These composite test cases have been used heavily in modernizing Coulomb functions, one of the basic building blocks of SAMMY. On careful comparison of results computed by the modern versus legacy Coulomb functions for the test cases involving a charged projectile, where differences were found it has been concluded that the modern Coulomb implementation yields more accurate results than the legacy Fortran implementation. Consequently, several of the composite test cases have been rebaselined using the modern Coulomb function, and these new results will serve as a baseline for future testing. In particular, the composite test cases that have been rebaselined are tr091, tr105, tr113, tr116, tr172, and tr177. Additional information about these test cases can be found in Table XII B.1 of the SAMMY Users' Guide [2].

In addition to the SAMMY test cases mentioned above, a brand new test case has been created to test the modern Coulomb function library directly. In this new test case, Coulomb functions are compared to values computed via known analytical expressions for the R-matrix shift and penetrability functions for electrically neutral particles. Furthermore, quad-precision values (i.e., 32 digits) of Coulomb functions for charge particles tabulated in the Table 2 of [9] for orbital angular momentum l=0 have been hard-coded into this test case. From those, Coulomb functions for l=1-5 have been computed by a recursion relation in [10]. This test case is now passing by a relative precision of  $10^{-8}$ , but on average the agreement is found to be much nearer to  $10^{-16}$  relative precision. Finally, a direct comparison to Coulomb functions implemented by Wolfram Mathematica 11.2 has revealed an excellent agreement with the modern Coulomb library, even for combinations of input parameters for which Coulomb functions are known to be inherently difficult to compute.

With the modern Coulomb function library, and with the changes described above, the SAMMY code has successfully passed all its nearly 190 composite test cases, including the new ones described above, and on the following OS/compiler combinations: (1) Mac/gcc, (2) Linux/gcc, and (3) Windows/ifort.

#### 11. SAMMY 8.2.0 RELEASE PROGRESS REPORT

ORNL has officially released SAMMY 8.1 via RSICC (rsicc.ornl.gov) as announced in the April 2017 RSICC newsletter. New features planned for the FY2019 SAMMY 8.2 release include:

- Incorporating a C++ modern Coulomb wave function library CWFCOMPLEX into SAMMY. (complete)
- Extending summation over channels to include closed channels that were ignored in the legacy code. (complete)
- Include closed channels when computing analytical derivatives of cross sections used for optimizing SAMMY *R*-matrix parameters. (complete)

- Correct the bugs in the I/O of ENDF files for charged particles, whether by making corrections to the legacy code or by linking to the modern C++ ENDF I/O AMPX library. (in progress)
- Enable conversion from formal *R*-matrix parameters to Brune's alternative *R*-matrix parameters. (complete)
- Update SAMMY documentation as needed. (in progress)
- To better leverage voluntary contributions to the SAMMY modernization process from SAMMY users worldwide, the application process for releasing the SAMMY code under an open source license was initiated. The application for the SAMMY open source release is currently pending the release of the Coulomb wave function library CWFCOMPLEX by Dr. Nicolas Michel under an ORNL variant of the open source license.

#### 12. MODERNIZATION OF SAMMY PHYSICS AND OPTIMIZATION METHODS

In the process of revisiting the mathematical and physical origins of methods implemented in the legacy code, several potentially useful new features have been revealed that may bring immediate new functionality in the modernized version of SAMMY and could provide a platform to expand SAMMY features. Revisited methods used by the legacy SAMMY include the following:

- 1. By default, the legacy SAMMY uses an energy-dependent boundary condition,  $B_c = S_c(E)$ , that introduces an approximation. This approximation is recommended in seminal papers on R-matrix theory [6]; however, it leads to some deviations from the formally exact cross sections. These deviations occur mostly in the valleys between resonant peaks, and they were revealed in comparison with other R-matrix codes. In FY2019, this approximation was removed by replacing the boundary condition by any energy-independent boundary conditions, such as  $B_c = -l_c$ , and by extending the summation over channels that are currently restricted to open channels to closed channels.
- 2. Alternatively, the energy-dependent boundary condition,  $B_c = S_c(E)$ , stated in item 1 above, could be made exact by an alternative or physical R-matrix parameterization derived by Prof. Carl Brune [11]. This alternative parameterization is appealing because the alternative resonance energies and widths closely correspond to positions and widths of the peaks visible in the cross sections.
- 3. The team has also derived analytical expressions for derivatives of *R*-matrix cross sections with regard to Brune's physical *R*-matrix resonance parameters. This will be necessary for fitting those parameters directly to measured cross-section data. (Alternatively, one could fit formal *R*-matrix parameters, as before, and convert to a physical *R*-matrix step at each Bayesian update to remove the need for implementing these analytical derivates.)

The following methods will be implemented in the future:

- The legacy code only fits one particle pair in the incoming channel at a time, when all possible incoming particle pairs leading to the same compound nuclear resonance should be fitted simultaneously.
- In the legacy code, only one normalization constant can be fitted by SAMMY, even when fitting more than one data set. Each data set should have its own normalization constant parameter.
- Bayesian parameter fitting method, also known as generalized least squares (GLS), was
  implemented in the legacy code. This method has been revisited, and a more general method has
  been derived for implementation of the Fit API [13]. The GLS method has now been
  implemented in a modernized framework for backward compatibility with the legacy code.

- In the process of revisiting the conventional Reich-Moore approximation (of the full R-matrix) implemented in SAMMY, a generalization of the Reich-Moore approximation has been derived. This transparently unitary generalization formally yields particle cross sections identically equal to those of the full R-matrix [14], and it may be considered for implementation in future versions of modernized SAMMY.
- A novel phenomenological parameterization of direct radiative capture has been proposed via the imaginary component of the *R*-matrix channel radius.

#### 13. SUCCESSION PLANNING

Over the past few years, the ever-growing list of graduate student summer interns (Jesse Brown, Jinghua Feng, Christopher Chapman<sup>3</sup>, and Amanda Youmans); one postdoctoral researcher (Andrew Holcomb<sup>4</sup>); and two research staff members (Vladimir Sobes and Marco Pigni) have become proficient SAMMY code users or developers.

During summer 2018, a Nuclear Engineering Science Laboratory Synthesis summer intern, **Jesse Brown**, has prototyped a new correction function to the neutron capture yield in the SAMMY code. Brown is a PhD graduate student of Prof. Yaron Danon in the Nuclear Engineering program at RPI. Brown's planned contributions to the SAMMY modernization effort may lead to a PhD thesis project that would train him for long-term development of nuclear data evaluation methods in the modernized SAMMY framework.

The work initiated in FY2017 by then-postdoctoral research associate **Dr. Andrew Holcomb**, who had translated the prototype GLS method implemented by Feng to conform to the Fit API of the modernized SAMMY framework, thus producing an important backward-compatible parameter optimization method, has been dormant during FY2018 due to changes in the modernization strategy. Work will be resumed at a later time. This and any other parameter optimization method that implements Fit API could be used by all other modules of SCALE and AMPX.

ORNL research staff members who contributed to the SAMMY 8.1 release in FY2017 are Drs. Vladimir Sobes and Dorothea Wiarda. **Dr. Sobes** has contributed the SAMINT module that fine-tunes mean values of *R*-matrix resonance parameters to achieve a better agreement between integral benchmark simulations and measurements [15], and he has created new SAMINT test cases. **Dr. Wiarda** has introduced the modern SQA of SCALE and AMPX to SAMMY, as well as robust methods for a piecemeal replacement of select legacy Fortran modules in SAMMY by their corresponding C++ API-based modernized modules, thus ensuring that legacy SAMMY results are reproduced by the modernized SAMMY code at each step of the modernization.

Following the SAMMY 8.1 release, **Dr. Marco Pigni** introduced summation over closed channels into the SAMMY implementation of cross-section calculations. This was necessary to enable comparison of cross sections computed by SAMMY with other *R*-matrix codes at the 4th International Atomic Energy Agency (IAEA) Consultants' Meeting described in Section 15.

**Dr. Chris Chapman** developed a thermal neutron scattering kernel evaluation capability that will be combined with the *R*-matrix resonance evaluation capability in SAMMY to enable first-time simultaneous fitting of *R*-matrix resonance parameters and thermal neutron scattering libraries. This will result in

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<sup>&</sup>lt;sup>3</sup> Dr. Chapman received his PhD from Georgia Institute of Technology for his work developing the thermal neutron scattering framework [16] and joined the Nuclear Data & Criticality Safety Group as a postdoctoral research associate.

<sup>&</sup>lt;sup>4</sup> Dr. Holcomb joined the Nuclear Data & Criticality Safety Group as a full-time research staff member.

improved consistency and covariance data between the two corresponding energy ranges. Thermal neutron scattering data were measured by the RPI researchers at ORNL's Spallation Neutron Source.

**Dr. Vladimir Sobes** prepared a hands-on *R*-matrix course for nuclear data evaluators that was recently conducted at RPI and the Massachusetts Institute of Technology to educate the new generation of nuclear engineers about the vital importance of nuclear data.

#### 14. SUMMARY AND PATH FORWARD

Development of features planned for SAMMY 8.2.0 release continued during FY2018 in a modern SQA and development framework shared with modernized SCALE and AMPX, enabling a modular API-based development of features in C++. This design decision will enable the modernized AMPX Resonance API to be leveraged for computation of cross sections by the modernized SAMMY.

In view of a change made in tactical approach to the SAMMY modernization effort to facilitate *incremental* modernization of SAMMY legacy features and implementation of new SAMMY features that would be available to nuclear data evaluators, in early in FY2018, new Fit API was designed for fitting *R*-matrix resonance parameters. The first implementation of Fit API has been the GLS for backward compatibility with the legacy SAMMY. During FY 2018 SAMMY 8.2 will be released with the following anticipated features:

- 1. An API has been created for Coulomb functions to enable transparent replacement of various Coulomb function implementations, such as Prof. Nicolas Michel's modern implementation when legacy implementations fail [8].
- 2. Summation over reaction channels has been expanded in SAMMY to include closed channels. This makes it consistent with *R*-matrix formalism, and it enables comparison with other R-matrix codes that include closed channels.
- 3. The Brune's transform [12] between formal and physical *R*-matrix parameters has been implemented.
- 4. A complete covariance matrix will be enabled for angular distributions of reaction channels currently not enabled in the legacy SAMMY code.
- 5. Distinct normalization coefficients will be enabled, one per data set, to fulfill a missing feature in the legacy code in which a single normalization coefficient has been used for all data sets.
- 6. Simultaneous fitting of R-matrix resonance parameters will be enabled. The parameters correspond to compound nuclear resonances that are reachable by various incoming particle pairs or various projectile-target pairs. This is another missing feature of the legacy SAMMY code. For example,  ${}^{7}$ Be compound resonances can be reached via protons incident on  ${}^{6}$ Li and via  $\alpha$ -particle incidents on  ${}^{3}$ He, both leading to the same compound resonant state. Contributions of direct reaction amplitudes, however, will be different in the two reactions.
- 7. An I/O API will be implemented that could read/write SAMMY input files for backward compatibility.

To the extent that time and funding allow, effects related to experimental conditions will be implemented in the modernized framework during FY 2019, including:

- Doppler broadening via Solbrig's kernel, ideally implemented using the fast Gauss transform,
- Resolution broadening as a convolution of various resolution functions for backward compatibility with the legacy SAMMY code,

- Modeling of the experimental background by parameterized functions, and
- High-fidelity modeling of experimental effects (e.g., multiple scattering) by seamless linking to ORNL's high-performance SHIFT Monte Carlo neutron transport code via its API.

With Doppler broadening of cross sections, and at least one experimental facility's<sup>5</sup> resolution functions implemented, work can begin to fit differential cross-section data, including experimental broadening. This would enable realistic fits to be performed completely within the modernized SAMMY framework.

In the process of revisiting the mathematical and physical origins of methods implemented in the legacy code, several potentially useful new features were discovered that may be implemented in the modernized framework. For example, revisiting the conventional application of Bayes' theorem to nuclear data evaluations in SAMMY led to a derivation of a new evaluation scheme that could be applied simultaneously to *R*-matrix resonance parameters and to parameters that define integral benchmark experiments (e.g., dimensions, material composition). This would optimize overall agreement with differential *and* integral measured data and would provide a simultaneous, consistent evaluation method of differential and integral data. In turn, this would yield a covariance of integral benchmark experiments. In addition to this benefit, this method is designed to account for any known model defects. The derivation of this method has been presented at and published in the proceedings of the 4<sup>th</sup> International Workshop on Nuclear Data Covariances (organized by CEA Cadarache and NEA, and held in Aix en Provence, France on October 2–6, 2017) [13]. The new method will be implemented in the modernized SAMMY via the Fit API described earlier.

To advertise SAMMY modernization efforts to the broader nuclear data community, team members contributed SAMMY-related sections to an IAEA-sponsored journal article in which results of several available *R*-matrix codes have been compared. Due to higher priorities elsewhere, there has been a temporary absence of activity during FY2018 in a collaboration with Prof. Dean W. Halderson of Western Michigan University initiated in FY2017 to consider accurate calculation of relativistic effects that may be useful for resonant cross-section evaluations of light nuclides for which RRR may extend into 10s of MeV, where relativistic effects may be tangible. This attempt would be the first to use Dirac relativistic *R*-matrix formalism in a nuclear data evaluation framework for improved precision and accuracy. This *R*-matrix formalism could be used in the modernized version of SAMMY.

Building on a successful defense of his PhD thesis ("Thermal Neutron Scattering Evaluation Framework," Georgia Institute of Technology, June 23, 2017), Chapman has been investigating the feasibility of using the Path Integral Molecular Dynamics (PIMD) method to account for nuclear quantum effects that have been neglected in extant thermal scattering libraries such as ENDF. The research team plans to use PIMD in FY2019 to evaluate water and other hydrogenous materials for which quantum effects are known to be significant. The feasibility of simultaneously evaluating thermal neutron scattering and *R*-matrix resonance parameters will also be investigated in the unified framework of modernized SAMMY.

### 15. TRAVEL AND CONFERENCES

At the Cross Section Evaluation Working Group, Nuclear Data Week, held at Brookhaven National Laboratory in November 2017, **Goran Arbanas** presented progress made to date in the effort to modernize SAMMY. The presentation highlighted recently developed features of the modernized SCALE/AMPX framework that continue to be leveraged by the modernized SAMMY code. A summary of the recent advances in ORNL nuclear data evaluation methodologies in the thermal and resolved

<sup>&</sup>lt;sup>5</sup> Resolution functions for, e.g., RPI, GELINA, ORELA, or n-TOF.

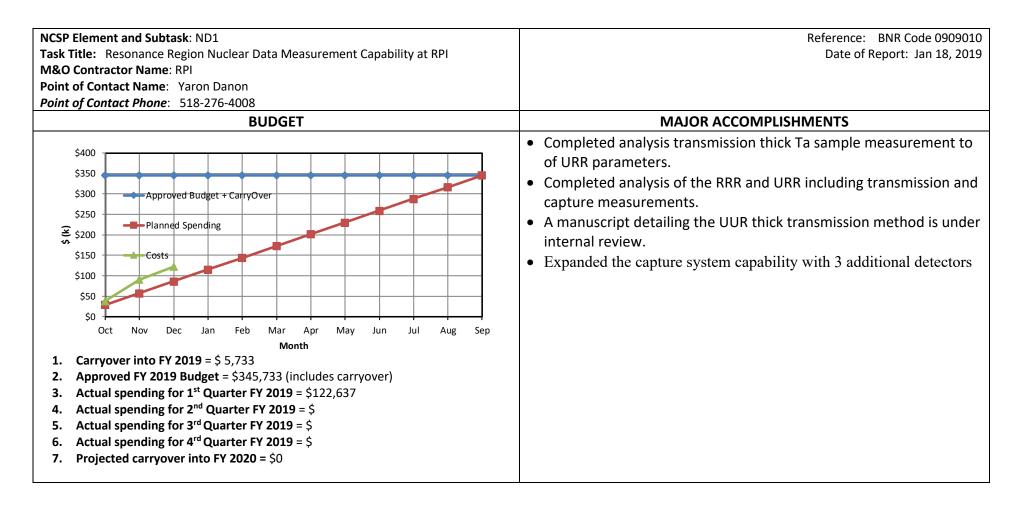
resonance regions have been presented. These advances will be implemented in the modernized version of the SAMMY code.

**Goran Arbanas** made a presentation ("Bayesian Optimization of Generalized Data") at the 4<sup>th</sup> International Workshop on Nuclear Data Covariances (CW2017), held in Aix En Provence, France, on October 2–6, 2017 (http://www.cw2017.com). The workshop was organized by the CEA and the NEA. These formal results will be incorporated into a new SAMMY API framework for nuclear data evaluations and have a potential to improve accuracy of uncertainties in nuclear data evaluations generally.

**Marco Pigni** participated in the 4th Consultants' Meeting on *R*-matrix Codes for Charged-particle Induced Reactions in the Resolved Resonance Region to compare angular differential cross sections computed by the SAMMY Code to other *R*-matrix codes for the <sup>7</sup>Be resonance analysis in p+<sup>6</sup>Li and <sup>3</sup>He+<sup>4</sup>He reactions. For more information, visit, https://www-nds.iaea.org/index-meeting-crp/CM\_R-matrix2018/.

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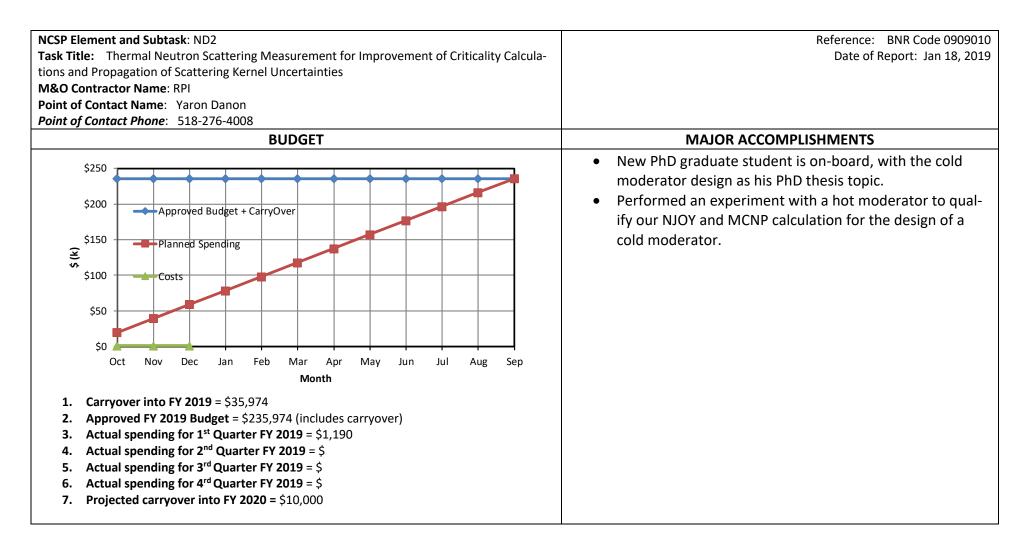


## RPI ND1 Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND1)		
	Provide status reports on RPI participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest. (ND1)		Nothing to report for Q1
	Complete analysis of measurement from FY18. (ND1)		
Q2	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND1)		
	Provide status reports on RPI participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest. (ND1)		
Q3	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND1)		
	Provide status reports on RPI participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest. (ND1)		
	Complete transmission measurement per the nuclear data schedule in Appendix B. (ND1)		Material for transmission was not selected; scattering measurements for Zr-nat are planned.
	Complete capture measurement per the nuclear data schedule in Appendix B. (ND1)		Material for capture was not selected; scattering measurements for Zr-nat are planned.
Q4	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND1)		·

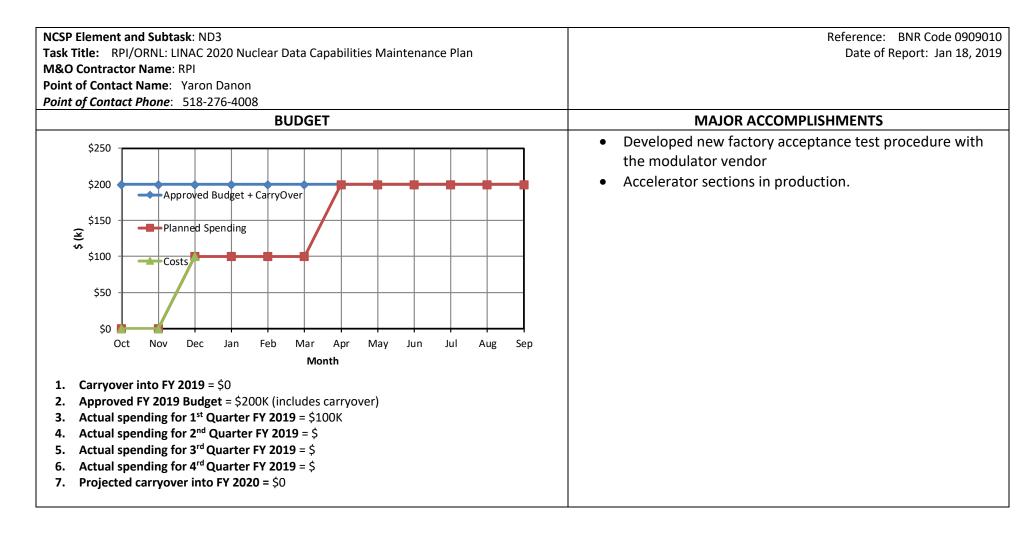
Provide status reports on RPI participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest. (ND1)	
Complete data analysis for transmission and capture measurements and provide the data to ORNL as needed to support the evaluation effort per the nuclear data schedule in Appendix B (ND1)	



## RPI ND2 Milestones:

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Complete	On Schedule	Behind Schedule	Missed Milestone

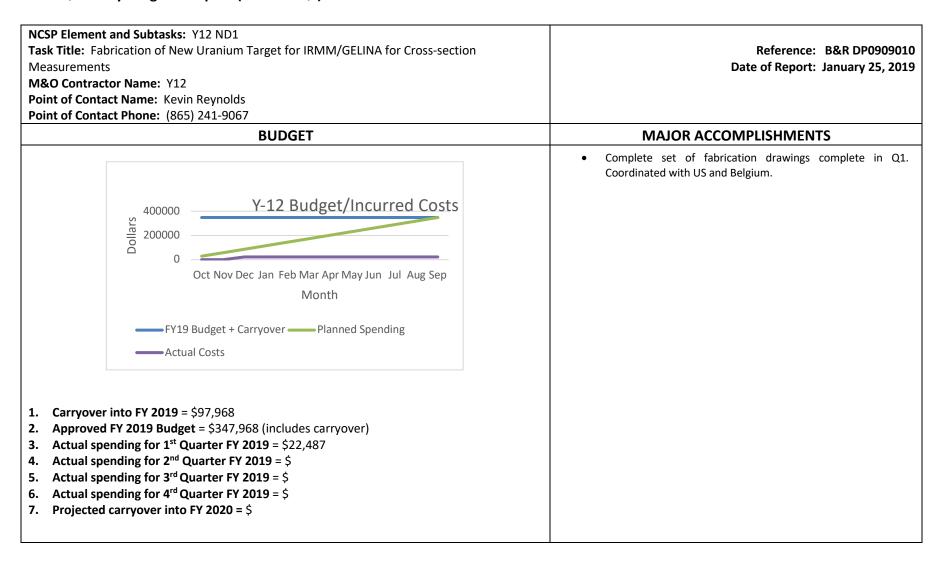
QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND2)		
	Provide status reports on RPI participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest (ND2)		Nothing to report in Q1
Q2	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND2)		
	Provide status reports on RPI participation in US and Interna- tional Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest (ND2)		
	Complete cold moderator preliminary design phase (ND2)		
Q3	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND2)		
	Provide status reports on RPI participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest (ND2)		
Q4	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND2)		
	Provide status reports on RPI participation in US and International Nuclear Data collaborations, and for foreign travel, provide a brief trip summary report to NCSP Manager on items of NCSP interest (ND2)		
	Complete cold moderator design (ND2)		



## RPI ND3 Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone

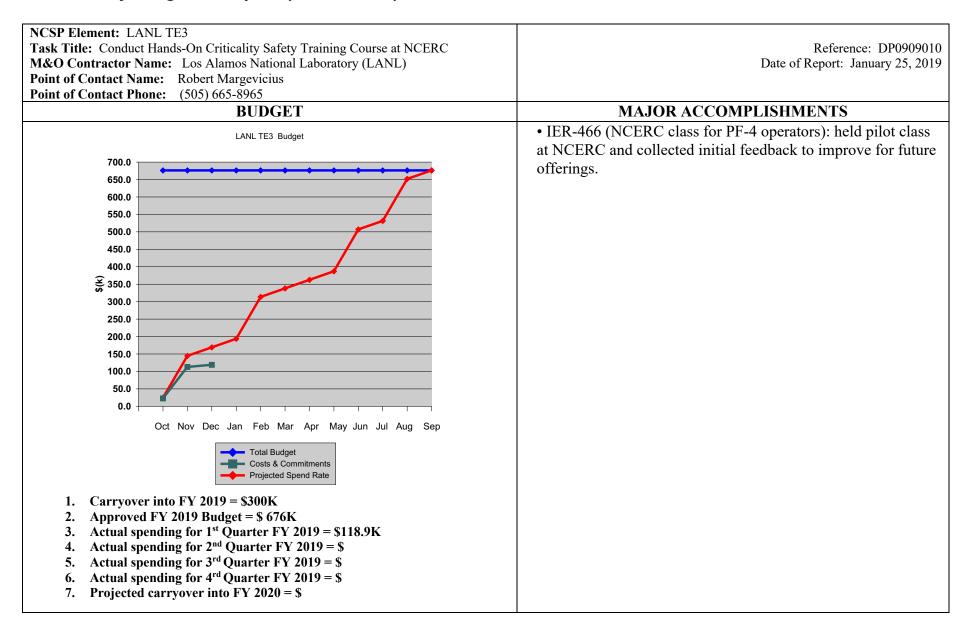
QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND3)		
	Factory acceptance tests of RF Modulators 2 and 3 (ND3)		Delay at the factory in Modulator 1, this is not the critical path, no impact on the target date is expected
Q2	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND3)		
	Delivery of RF Modulator 1 and Klystron 1 (ND3)		Expected cascade of the above
	Factory acceptance tests of RF Modulators 4 and 5 (ND3)		Expected cascade of the above
Q3	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND3)		
	Factory Acceptance test for Tapered Phase Velocity and Speed of Light #1 Accelerator Sections (ND3)		
Q4	Provide status reports on all nuclear data support activities in NCSP Quarterly Progress Reports. (ND3)		
	Delivery and of TPV and SOL1 Accelerator Sections (ND3)		



## Y12 ND Milestones:

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	Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	COMMENTS
Q1	Provide a status report of the fabrication of a depleted uranium/molybdenum target per IRMM/GELINA specifications to the NCSP Manager. (ND1)		Fabrication of part to commence in Q2
Q2	Provide a status report of the fabrication of a depleted uranium/molybdenum target per IRMM/GELINA specifications to the NCSP Manager. (ND1)		
Q3	Provide a status report of the fabrication of a depleted uranium/molybdenum target per IRMM/GELINA specifications to the NCSP Manager. (ND1)		
Q4	Provide a status report of the fabrication of a depleted uranium/molybdenum target per IRMM/GELINA specifications to the NCSP Manager. (ND1)		



### LANL TE3 Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone
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QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports on all training activities to the NCSP		
	Manager. (TE3)		
	Provide training in accordance with the approved schedule. (TE3)		
Q2	Provide status reports on all training activities to the NCSP Manager. (TE3)		
	Provide training in accordance with the approved schedule. (TE3)		
Q3	Provide status reports on all training activities to the NCSP Manager. (TE3)		
	Provide training in accordance with the approved schedule. (TE3)		
Q4	Provide status reports on all training activities to the NCSP Manager. (TE3)		
	Provide training in accordance with the approved schedule. (TE3)		

NCSP Element: LANL TE4 Task Title: On-Site Introductory Training for the NCS Practitioner on Modern Reference: B&R DP0909010 Approaches to Validation using Sensitivity and Uncertainty Analysis Tools Date of Report: January 24, 2019 **M&O Contractor Name:** Los Alamos National Laboratory (LANL) Point of Contact Name: Robert Margevicius / Bob Little **Point of Contact Phone:** (505) 665-8965 / (505) 665-3487 **BUDGET** MAJOR ACCOMPLISHMENTS Sensitivity / Uncertainty Workshop scheduled for February 35 13-14 at Hanford. 30 25 20 Costs ♣ Planned Spending 15 → Approved Budget 10 5 Jan Feb Mar Apr May Jun 1. Carryover into FY 2019 = \$0Approved FY 2019 Budget = \$30,000 (includes carryover) 3. Actual spending for 1st Quarter FY 2019 = \$0 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$ Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$ Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$ 7. Projected carryover into FY 2020 = \$0

### LANL TE4 Milestones:

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Complete	On Schedule	Behind Schedule	Missed Milestone

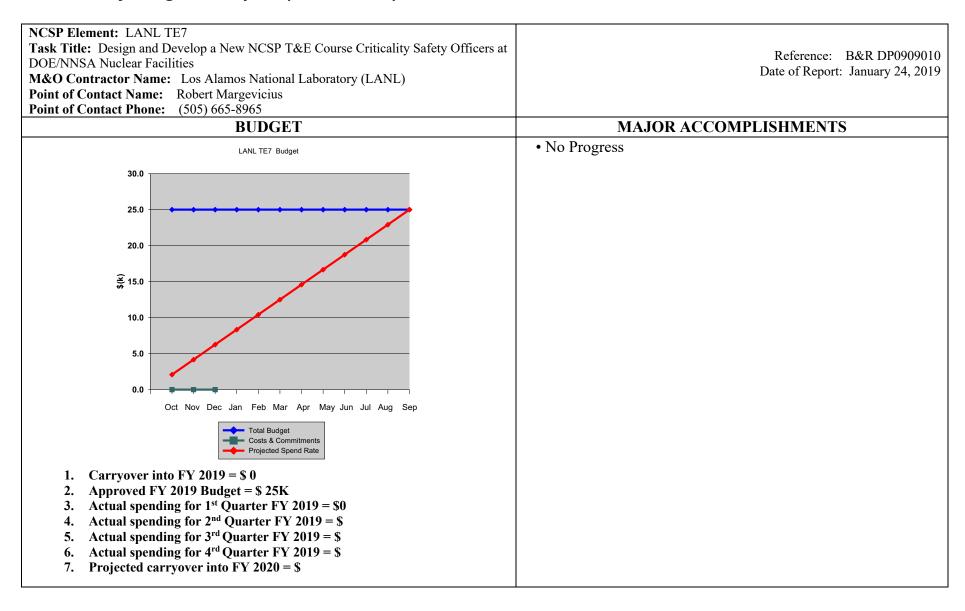
QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	NONE		
Q2	NONE		
Q3	NONE		
Q4	In collaboration with ORNL, provide introductory 1-day S/U workshop training to one or more DOE sites in FY19. (TE4)		

NCSP Element: LANL TE6 Task Title: Development of University Pipeline for Criticality Safety Professionals M&O Contractor Name: Los Alamos National Laboratory (LANL) Point of Contact Name: Robert Margevicius Point of Contact Phone: (505) 665-8965  BUDGET	Reference: B&R DP0909010 Date of Report: January 25, 2019  MAJOR ACCOMPLISHMENTS
1. Carryover into FY 2019 = \$0 2. Approved FY 2019 Budget = \$ 92K 3. Actual spending for 1st Quarter FY 2019 = \$0 4. Actual spending for 2nd Quarter FY 2019 = \$ 5. Actual spending for 3rd Quarter FY 2019 = \$ 6. Actual spending for 4rd Quarter FY 2019 = \$ 7. Projected carryover into FY 2020 = \$ 7. Projected carryover into FY 2020 = \$ 7. Projected carryover into FY 2020 = \$ 7.	No Progress

## **LANL TE6 Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

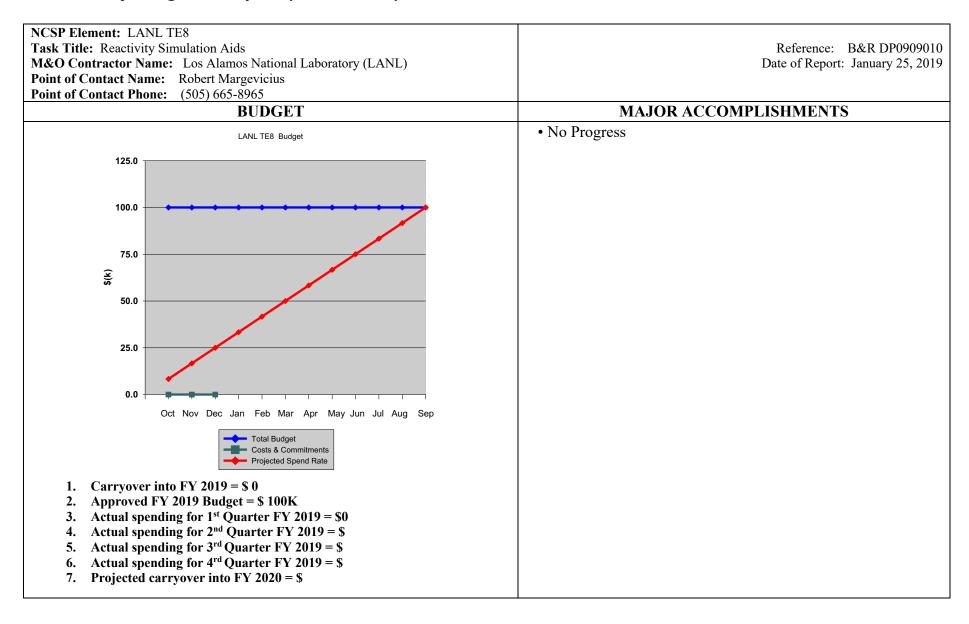
QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports on all training activities to the NCSP Manager. (TE6)		Will work with NCSD to plan strategy.
Q2	Provide status reports on all training activities to the NCSP Manager. (TE6)		
Q3	Provide status reports on all training activities to the NCSP Manager. (TE6)		
Q4	Provide status reports on all training activities to the NCSP Manager. (TE6)		
	Provide end of year progress report. (TE6)		



### LANL TE7 Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone
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QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports on all training activities to the NCSP Manager. (TE7)		
Q2	Provide status reports on all training activities to the NCSP Manager. (TE7)		
Q3	Provide status reports on all training activities to the NCSP Manager. (TE7)		
Q4	Provide status reports on all training activities to the NCSP Manager. (TE7)		
	Provide end of year progress report. (TE7)		



### LANL TE8 Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone
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QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports on all training activities to the NCSP Manager. (TE8)		Will work with NCSD to plan work.
Q2	Provide status reports on all training activities to the NCSP Manager. (TE8)		
Q3	Provide status reports on all training activities to the NCSP Manager. (TE8)		
Q4	Provide status reports on all training activities to the NCSP Manager. (TE8)		
	Provide end of year progress report. (TE8)		

NCSP Element and Subtasks: TE1, 3, 8, 9

Task Titles:

- TE1 Conduct Hands-on Training at the DAF (TACS)
- TE3 Classroom Criticality Safety Training
- TE8 Incorporate Superior Reflectors into TACS "Hands On" Training
- TE9 Design and Develop a New NCSP T&E Course for Criticality Safety Officers

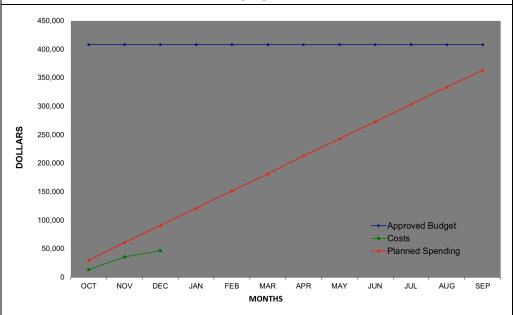
**M&O Contractor Name:** Lawrence Livermore National Laboratory

**Point of Contact Name:** David Heinrichs **Point of Contact Phone:** (925) 424-5679

Reference: B&R DP0909010

Date of Report: January 25, 2019

### BUDGET



- 1. Carryover into FY 2019 = \$12,541
- Approved FY 2019 Budget = \$408,541 (includes carryover)
- 3. Actual spending for 1st Quarter FY 2019 = \$47,065
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$
- 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$
- 7. Projected carryover into FY 2020 = \$12,541 (11%)

### MAJOR ACCOMPLISHMENTS

- 1. Provided registration and logistics support (TE1, TE3) for:
  - 2-week CSE course on Jan 28-Feb 8, 2019 at NATM & NCERC/SNL
  - 1 week Managers course on April 8-12, 2019 at SNL
  - 1 week Managers course on June 3-7, 2019 at NCERC
  - 2-week CSE course on Aug 12-23, 2019 at NATM & NCERC/SNL
- 2. Participated in a face-to-face T&E two-day meeting at ORNL on October 17-18, 2018 to review and update 1<sup>st</sup> week course materials (TE1, TE3).
- 3. Participated in all T&E teleconferences (TE1, TE3).
- 4. The CSE for adding Be to the TACS is in final review and scheduled for completion next quarter (TE8).
- Provided the LLNL response to a CSSG questionnaire issued October 29, 2018 for information regarding a "Potential Class on Improving Effectiveness of NCS Interface with Operations/ Production" on November 6, 2018 (TE9).

### **LLNL T&E Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	COMMENTS
Q1	Update, maintain and support the registration process and provide classroom and "hands on" TACS training in accordance with the schedule approved by the NCSP Manager (TE1, TE3).		
	Conduct subcritical measurements using beryllium shells and finalize training materials addressing the concept of superior reflection. (TE8)		CSE in final review.
	Provide a status report of the status of efforts to develop a new CSO/FMH course for the NCSP for piloting in FY20. (TE9)		Provided LLNL response to CSSG questionnaire.
Q2	Update, maintain and support the registration process and provide classroom and "hands on" TACS training in accordance with the schedule approved by the NCSP Manager (TE1, TE3).		
	Conduct subcritical measurements using beryllium shells and finalize training materials addressing the concept of superior reflection. (TE8)		
	Provide a status report of the status of efforts to develop a new CSO/FMH course for the NCSP for piloting in FY20. (TE9)		
Q3	Update, maintain and support the registration process and provide classroom and "hands on" TACS training in accordance with the schedule approved by the NCSP Manager (TE1, TE3).		
	Conduct subcritical measurements using beryllium shells and finalize training materials addressing the concept of superior reflection. (TE8)		
	Provide a status report of the status of efforts to develop a new CSO/FMH course for the NCSP for piloting in FY20. (TE9)		
Q4	Update, maintain and support the registration process and provide classroom and "hands on" TACS training in accordance with the schedule approved by the NCSP Manager (TE1, TE3).		
	Conduct subcritical measurements using beryllium shells and finalize training materials addressing the concept of superior reflection. (TE8)		
	Provide a status report of the status of efforts to develop a new CSO/FMH course for the NCSP for piloting in FY20. (TE9)		

NCSP Element and Subtask: TE1, 5, 9, 10

Task Title: See last page
M&O Contractor Name: ORNL
Point of Contact Name: Doug Bowen
Point of Contact Phone: (865) 576-0315

Reference: DP0909010/ORNL Date of Report: January 20, 2019

### BUDGET

# FY19 Training and Education 400 350 300 250 250 100 50 Oct Nov Dec Jan Feb Mar Apr May Jun Jul Aug Sep Approved Budget Planned Spending

- 1. Carryover into FY19 = \$40K
- 2. Approved Budget FY19 = \$374K (includes carryover)
- 3. Actual spending for 1st Quarter FY19 = \$37K
- 4. Actual spending for 2nd Quarter FY19
- 5. Actual spending for 3rd Quarter FY19
- 6. Actual spending for 4th Quarter FY19

### **MAJOR ACCOMPLISHMENTS**

# TE1 - Manage and Provide Instruction for the DOE Nuclear Criticality Safety Training & Education Program

- 2016-01 assessment documentation completed and archived.
   All comments from the 2016-01 CSSG assessment have been dispositioned.
- Archived all FY2018 records on the NCSP Training and Education SharePoint, i.e., exams, photographs, course materials, and student evaluation forms.
- Arranged an conducted a FY2019 face-to-face meeting with the core faculty for the 1<sup>st</sup> week of the 2-week hands-on course (Hicks, Bowen, Percher, Haught, Lousteau, Marshall, & Adams). The course agenda, materials, and, especially, the CSE workshops were discussed and enhanced. Assignments were issued to all participants to modify the course materials for the Feb. 2019 course. Some modifications are pending some other changes and will be completed for the Aug. 2019 course.
- Lousteau has been trained to replace Jeff Chapman as the NDA instructor for the course. Jeff has participated in the 2week hands-on course since 2011.
- ORNL instructors updated course modules per the plan generated in October 2018. The introduction, DOE module, standards, and workshop slides were modified.
- Late in Q1, telecons to prepare for the 2-week hands-on course were planned and conducted.

# TE5 - On-Site Introductory Training for the NCS Practitioner on Modern Approaches to Validation using Sensitivity and Uncertainty Analysis Tools

 Worked with LANL (Brown, Alwin, Rising) and with Hanford (Alyssa Kersting) to schedule, plan, and arrange the next S/U course. This is currently scheduled over a 2-day period due to the needs of two organizations at Hanford. 12-18 students plan to attend. The course will be located at the HAMMER facility in North Richland and will be conducted Feb. 13-14, 2019.

NCSP Element and Subtask: TE1, 5, 9, 10 Task Title: See last page M&O Contractor Name: ORNL Point of Contact Name: Doug Bowen Point of Contact Phone: (865) 576-0315	Reference: DP0909010/ORNL Date of Report: January 20, 2019
T diff of Contact Findic. (003) 370-0013	<ul> <li>TE9 - Design and Develop a New NCSP T&amp;E Course for Criticality Safety Officers at DOE/NNSA Nuclear Facilities</li> <li>This task is pending completion of the 2018-01 CSSG tasking report. At the time of this report, the tasking report has been drafted and has been sent out for review amongst the CSSG CSO training course team. Anticipate the actual design work starting in mid- to late-Q2.</li> <li>TE10 - Design of a Subcritical Assembly at ORNL for use with the CSO/FMH Courses</li> <li>Computations have been initiated for this task. Multiple AGN 201 core pieces have been located at Y-12. Q2 work will be to identify a complete set of fuel plates for use at ORNL for the subcritical assembly. A design report will be completed in Q4 for the sake of an FY2021 proposal to continue the development of a prototype for subcritical measurements at ORNL. ORNL management have provided \$80k in program development funds to explore a facility location for the subcritical assembly once it is constructed. Local universities have expressed great interest in this new facility/capability that is being explored at ORNL.</li> </ul>

### **ORNL TE Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide a status report in NCSP Quarterly Progress Reports on implementation of the NCS training program and resolution of CSSG comments from CSSG tasking 2016-01. (TE1)		
	Provide status reports in NCSP Quarterly Progress Reports on improvements/modifications to baseline NCS course training materials based on CSSG assessment report 2016-01, self-evaluation, and feedback from reviewers, observers, trainers, and the NCSP manager. (TE1)		
	Provide a status report in NCSP Quarterly Progress Reports on the progress of 1-day onsite introductory validation training conducted at one or more DOE sites. (TE5)		
	Provide a status report of the status of efforts to develop a new CSO/FMH course for the NCSP for piloting in FY20. (TE9)		
Q2	Provide a status report in NCSP Quarterly Progress Reports on implementation of the NCS training program and resolution of CSSG comments from CSSG tasking 2016-01. (TE1)		
	Provide status reports in NCSP Quarterly Progress Reports on improvements/modifications to baseline NCS course training materials based on CSSG assessment report 2016-01, self-evaluation, and feedback from reviewers, observers, trainers, and the NCSP manager. (TE1)		
	Provide a status report in NCSP Quarterly Progress Reports on the progress of 1-day onsite introductory validation training conducted at one or more DOE sites. (TE5)		
	Provide a status report of the status of efforts to develop a new CSO/FMH course for the NCSP for piloting in FY20. (TE9)		

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Q3	Provide a status report in NCSP Quarterly Progress Reports on im-	
	plementation of the NCS training program and resolution of CSSG	
	comments from CSSG tasking 2016-01. (TE1)	
	Provide status reports in NCSP Quarterly Progress Reports on im-	
	provements/modifications to baseline NCS course training mate-	
	rials based on CSSG assessment report 2016-01, self-evaluation,	
	and feedback from reviewers, observers, trainers, and the NCSP	
	manager. (TE1)	
	Provide a status report in NCSP Quarterly Progress Reports on the	
	progress of 1-day onsite introductory validation training con-	
	ducted at one or more DOE sites. (TE5)	
	Provide a status report of the status of efforts to develop a new	
	CSO/FMH course for the NCSP for piloting in FY20. (TE9)	
Q4	Provide a status report in NCSP Quarterly Progress Reports on im-	
	plementation of the NCS training program and resolution of CSSG	
	comments from CSSG tasking 2016-01. (TE1)	
	Provide status reports in NCSP Quarterly Progress Reports on im-	
	provements/modifications to baseline NCS course training mate-	
	rials based on CSSG assessment report 2016-01, self-evaluation,	
	and feedback from reviewers, observers, trainers, and the NCSP	
	manager. (TE1)	
	Provide a status report in NCSP Quarterly Progress Reports on the	
	progress of 1-day onsite introductory validation training con-	
	ducted at one or more DOE sites. (TE5)	
	Provide a status report of the status of efforts to develop a new	
	CSO/FMH course for the NCSP for piloting in FY20. (TE9)	
	Develop a feasibility report to the NCSP manager for the design	
	and installation of a subcritical assembly at ORNL using existing	
	resources at Y-12. If the concept is feasible, submit a proposal for	
	consideration for FY20. (TE10)	

### Task Title:

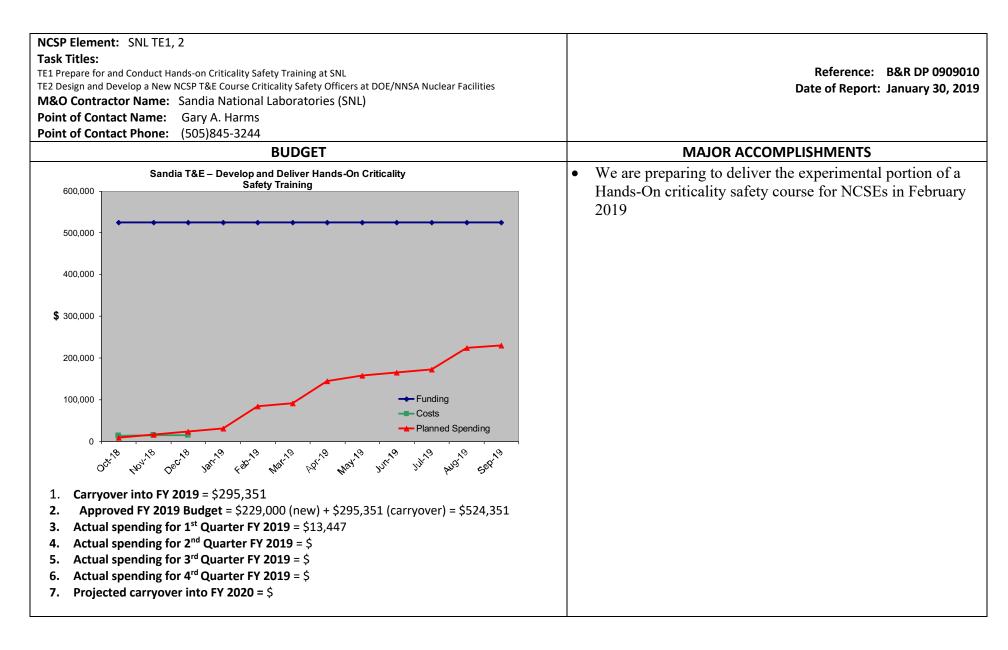
TE9

TE1 Manage and Provide Instruction for the DOE Nuclear Criticality Safety Training & Education Program

TE5 On-Site Introductory Training for the NCS Practitioner on Modern Approaches to Validation using Sensitivity and Uncertainty Analysis Tools

Design and Develop a New NCSP T&E Course for Criticality Safety Officers at DOE/NNSA Nuclear Facilities

TE10 Design of a Subcritical Assembly at ORNL for use with the CSO/FMH Courses



### SNL T&E Milestones:

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On Schedule	Behind Schedule	Missed Milestone			
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QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Conduct hands-on training classes at Sandia and provide Human		
	Factors and Equipment Reliability module support to the LANL		
	training classes in accordance with the approved schedule. (TE1)		
	Work with LLNL, ORNL, LANL to develop and deploy a 1-week		
	hands-on NCSP T&E course for fissile material handlers and		
	criticality safety officer. (TE2)		
Q2	Conduct hands-on training classes at Sandia and provide Human		
	Factors and Equipment Reliability module support to the LANL		
	training classes in accordance with the approved schedule. (TE1)		
	Work with LLNL, ORNL, LANL to develop and deploy a 1-week		
	hands-on NCSP T&E course for fissile material handlers and		
	criticality safety officer. (TE2)		
Q3	Conduct hands-on training classes at Sandia and provide Human		
	Factors and Equipment Reliability module support to the LANL		
	training classes in accordance with the approved schedule. (TE1)		
	Work with LLNL, ORNL, LANL to develop and deploy a 1-week		
	hands-on NCSP T&E course for fissile material handlers and		
	criticality safety officer. (TE2)		
Q4	Conduct hands-on training classes at Sandia and provide Human		
	Factors and Equipment Reliability module support to the LANL		
	training classes in accordance with the approved schedule. (TE1)		
	Work with LLNL, ORNL, LANL to develop and deploy a 1-week		
	hands-on NCSP T&E course for fissile material handlers and		
	criticality safety officer. (TE2)		

### NCSP Element and Subtasks: Y12 TE1, 3, 4 Task Title: Reference: B&R DP0909010 TE1 Conduct Hands-On Criticality Safety Training Course (Lecture support week 1 of 2-week hands-on course and Date of Report: January 25, 2019 course material development) TE3 Design of a Subcritical Assembly at ORNL for use with the CSO Courses TE4 Design and Develop a New NCSP T&E Course for Criticality Safety Officers at DOE/NNSA Nuclear Facilities **M&O Contractor Name:** Y12 Point of Contact Name: Kevin Reynolds Point of Contact Phone: (865) 241-9067 **BUDGET** MAJOR ACCOMPLISHMENTS TE1 is Chris Haught's time to teach at TAMU and Hands On Courses. Minimal effort in Q1 - mostly prep for TAMU teaching which is to occur in Q2. TE3 and TE4 are ORNL tasks we fund as requested and so far Y-12 Budget/Incurred Costs 200000 no effort from us on these items has occurred. Dollars 100000 Oct Nov Dec Jan Feb Mar Apr May Jun Jul Aug Sep Month FY19 Budget + Carryover —— Planned Spending —Actual Costs 1. Carryover into FY 2019 = \$0 2. Approved FY 2019 Budget = \$134k (includes carryover) Actual spending for 1st Quarter FY 2019 = \$5000 Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$ Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$ 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$ 7. Projected carryover into FY 2020 = \$

### Y12 TE Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	COMMENTS
Q1	Conduct hands-on training classes at NFO and NCERC to support the training classes in accordance with the approved schedule. (TE1, TE3, TE4)		
Q2	Conduct hands-on training classes at NFO and NCERC to support the training classes in accordance with the approved schedule. (TE1, TE3, TE4)		
Q3	Conduct hands-on training classes at NFO and NCERC to support the training classes in accordance with the approved schedule. (TE1, TE3, TE4)		
Q4	Conduct hands-on training classes at NFO and NCERC to support the training classes in accordance with the approved schedule. (TE1, TE3, TE4)		

NCSP Element and Subtask: TS1
Task Title: CSSG Support

M&O Contractor Name(s): AECOM, ANL, LANL, LLNL, PNNL, SRNS, Y-12

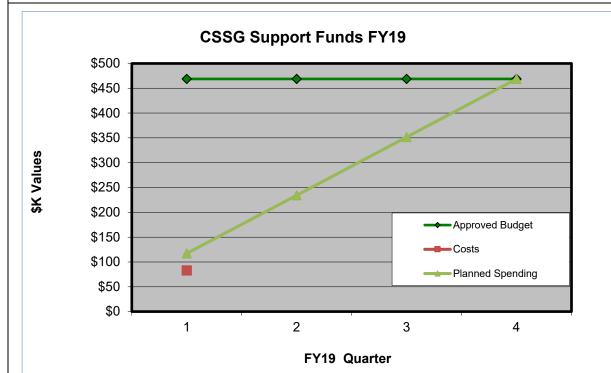
Point of Contact Name: David Hayes (CSSG Deputy Chair)

Point of Contact Phone: 505-667-4523

Reference: B&R DP 0909010

Date of Report: Jan 20, 2019

### **BUDGET**



- 1. Carryover into FY 2019 = \$k 48.8
- 2. Approved FY 2019 Budget = \$k 468.8 (includes carryover)
- 3. Actual spending for 1st Quarter FY 2019 = \$k 82.8
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$k
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$k
- 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$k
- 7. Projected carryover into FY 2020 = \$ 0

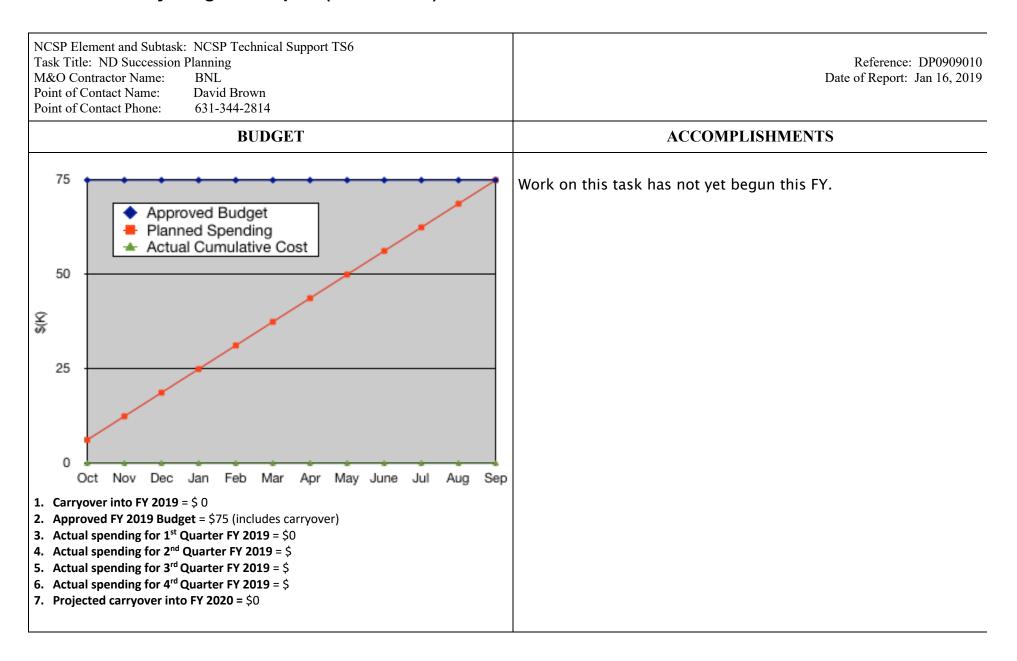
### MAJOR ACCOMPLISHMENTS

- Tasking 2018-01 ongoing
- CSSG Face-to-Face meeting in Orlando
- Regular CSSG Telecons

### **CSSG TS Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

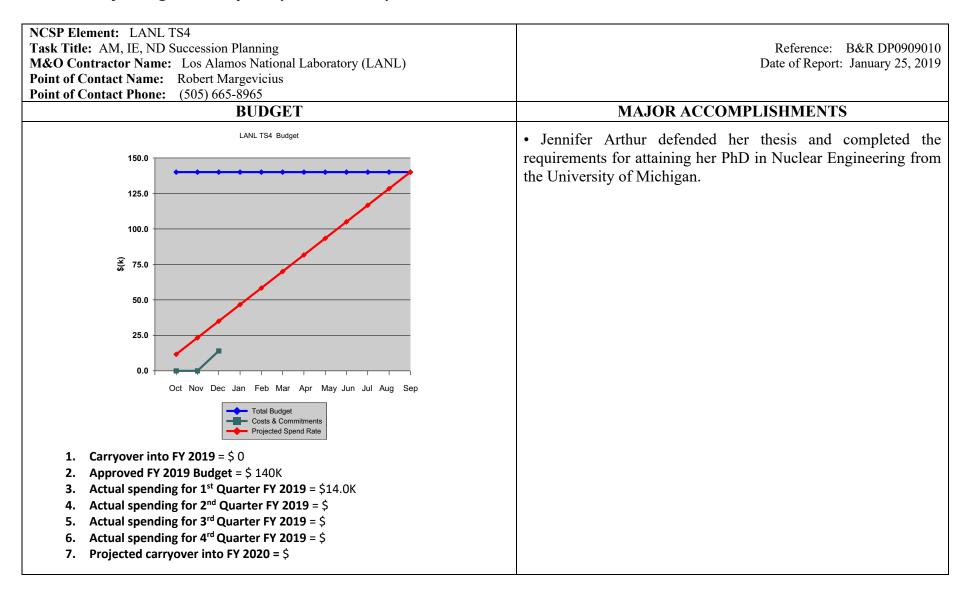
QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide the NCSP manager with a summary of CSSG activities, meetings, and tasks. (TS1)		Tasking 2018-01 not complete. Team refocused with expected completion by end of Q2.
Q2	Provide the NCSP manager with a summary of CSSG activities, meetings, and tasks. (TS1)		
Q3	Provide the NCSP manager with a summary of CSSG activities, meetings, and tasks. (TS1)		
Q4	Provide the NCSP manager with a summary of CSSG activities, meetings, and tasks. (TS1)		



### **BNL TS6 Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	NONE		n/a
Q2	NONE		
Q3	NONE		
Q4	Provide NCSP Manager annual report of succession planning efforts.		



### LANL TS4 Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	NONE		
Q2	NONE		
Q3	NONE		
Q4	Provide NCSP Manager annual report of succession planning efforts.		

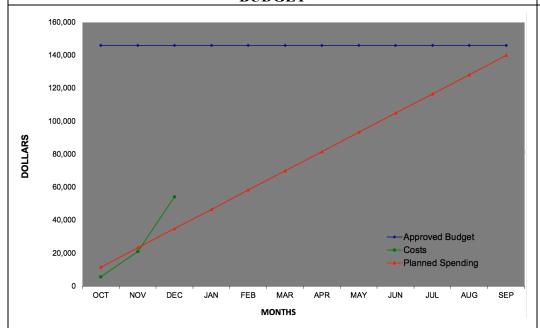
NCSP Element and Subtasks: TS5
Task Title: LLNL Succession Planning

M&O Contractor Name: Lawrence Livermore National Laboratory

**Point of Contact Name:** David Heinrichs **Point of Contact Phone:** (925) 424-5679

**Reference:** B&R DP0909010 **Date of Report:** January 25, 2019

### BUDGET



- 1. Carryover into FY 2019 = \$6,086
- 2. Approved FY 2019 Budget = \$146,086 (includes carryover)
- 3. Actual spending for 1st Quarter FY 2019 = \$54,353
- 4. Actual spending for 2<sup>nd</sup> Quarter FY 2019 = \$
- 5. Actual spending for 3<sup>rd</sup> Quarter FY 2019 = \$
- 6. Actual spending for 4<sup>rd</sup> Quarter FY 2019 = \$
- **7. Projected carryover into FY 2020 =** \$6,086 (4%)

### **MAJOR ACCOMPLISHMENTS**

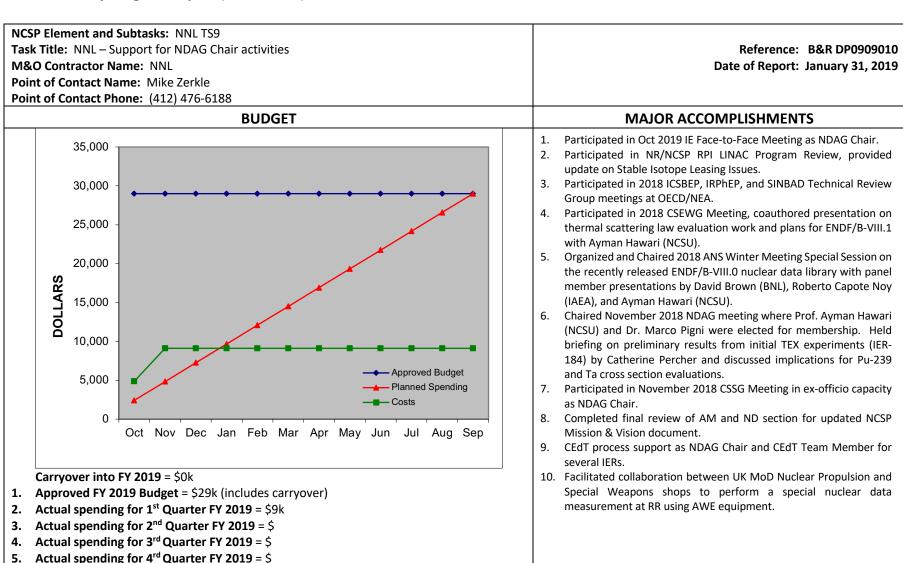
- 1. Provided LLNL-AR-759758, "LLNL NCSP Succession Planning Efforts in FY-2018," to the NCSP Manager on October 11, 2018.
- 2. Jim Reus selected to succeed John Scorby as technical SME for multiphysics methods (AM).
- 3. Caleb Mattoon succeeds Dave Brown (BNL) in developing energy dependent probability distribution functions for the unresolved resonance region in FUDGE/GND (AM).
- 4. Tony Nelson attended the 2018 IEEE Nuclear Science Symposium in Sydney, Australia on November 10-17, 2018 (IE, ND).
- 5. Tim Classen succeeds Nathaniel Bowden as technical SME for the hybrid neutron time-of-flight spectrometer (IE, ND).
- 6. Chuck Lee retired from LLNL on Dec. 4, 2018. Stacy Peterson succeeds him as NCSP and NDA website developer (IPD).
- 7. Tony Nelson participated in the October 22, 2018 ICSBEP meeting as a new evaluator (and reviewer) increasing the number of active LLNL evaluators to four (Biswas, Heinrichs, Kim, Nelson) (IPD).
- 8. Tony Nelson assisting Percher in updating the CSE supporting TACS "hands on" training including use of "superior" beryllium reflectors (T&E).

### LLNL TS5 Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	NONE		
Q2	NONE		
Q3	NONE		
Q4	Provide NCSP Manager annual report of succession planning efforts.		

Projected carryover into FY 2020 = \$ (0%)



### NNL TS9 Milestones:

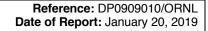
On Schedule	Behind Schedule	Missed Milestone
	On Schedule	On Schedule Behind Schedule

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD	
Q1	Provide the NCSP manager with a summary of NDAG chair activities, meetings, and tasks. (TS9)			
Q2	Provide the NCSP manager with a summary of NDAG chair activities, meetings, and tasks. (TS9)			
Q3	Provide the NCSP manager with a summary of NDAG chair activities, meetings, and tasks. (TS9)			
Q4	Provide the NCSP manager with a summary of NDAG chair activities, meetings, and tasks. (TS9)			

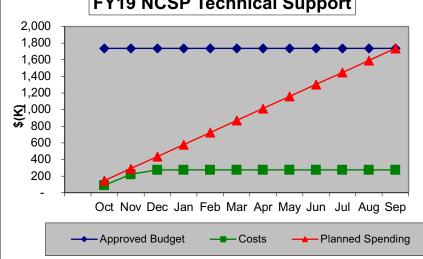
NCSP Element and Subtask: TS2 (NCSP Technical Support), TS7 (Succession Planning), TS8 (NCSP MGT Tool Development), TS11 (CEdT Manager Support)

**BUDGET** 

M&O Contractor Name: ORNL Point of Contact Name: Doug Bowen **Point of Contact Phone: (865) 576-0315** 



# **FY19 NCSP Technical Support**



- **1. Carryover into FY19 = \$613k**
- 2. Approved Budget FY19 = \$1,737K (includes carryover)
- 3. Actual spending for 1st Quarter FY19 = \$275K
- 4. Actual spending for 2nd Quarter FY19
- 5. Actual spending for 3rd Quarter FY19
- 6. Actual spending for 4th Quarter FY19

### TS2

Prepare and maintain elements of NCSP Plan and associated activities:

MAJOR ACCOMPLISHMENTS

- Monitor Five-Year Plan progress,
- Review/revise task list, and
- Schedule/participate in meetings and teleconferences.
- Manage and provide oversight/coordinate efforts for the NCSP Information, Preservation, and Dissemination task element.
- Manage and provide oversight/coordinate efforts for the NCSP Training and Education Program task element.
- Participated in NCSP management team and other NCSP-related meetings, as required by the NCSP Manager.
- Prepared Q4 QPRs into a single bookmarked PDF file for use in QPR. Conducted Q4 telecon.
- Published the summer/fall 2018 NCSP newsletter
- Worked with Mission and Vision team leads to complete their draft Mission and Vision sections. Compiled final draft of the document.
- Completed draft main and IE 5-year plans for FY19.
- Participated in CSSG telecons and assisted with CSSG tasks as necessary. Doug Bowen supporting CSSG tasking 2018-01 CSO course baseline.
- Finalized efforts to improve documentation of NCSP accomplishments to ensure NCSP work is linked to final 5YP milestones. Lori Scott has created new quarterly reporting templates for distribution to the site task managers.
- Led and participated in IE WebEx meetings in October and December

### TS7

• Chris Chapman continued to work on nuclear data evaluations with Vlad Sobes as a mentor, in particular, the Ce nuclear data evaluations. Chris is also working on thermal neutron scattering measurements at the ORNL SNS. Andrew Holcomb continued working on tasks to utilize SAMMY and AMPX for NCSP projects. Started planning for a new Nuclear Data Post-Doc to be brought onto the team Q2.

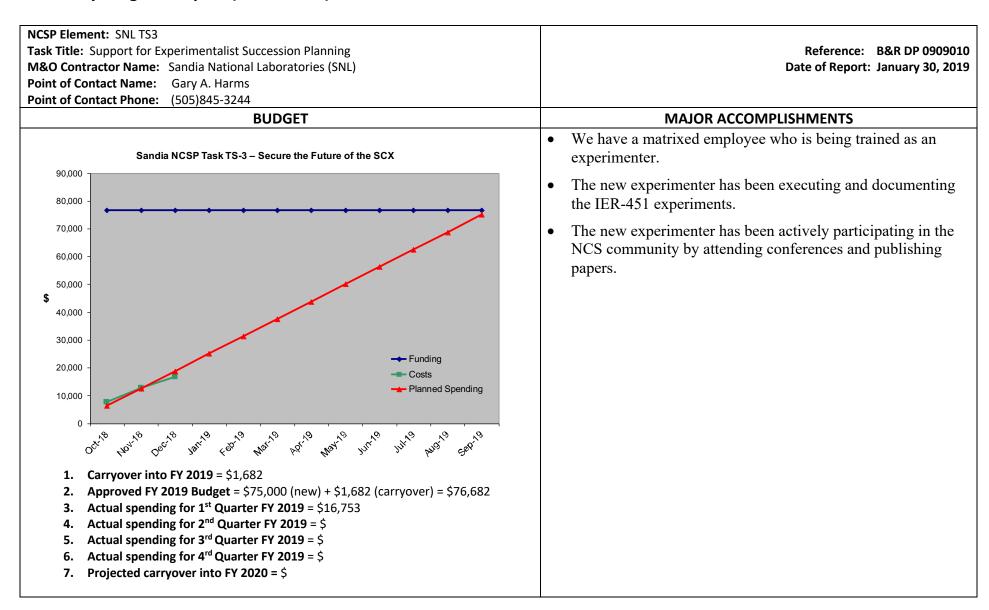
NCSP Element and Subtask: TS2 (NCSP Technical Support), TS7 (Succession Planning), TS8 (NCSP MGT Tool Development), TS11 (CEdT Manager Support) M&O Contractor Name: ORNL Point of Contact Name: Doug Bowen Point of Contact Phone: (865) 576-0315	Reference: DP090010/ORNL Date of Report: January 20, 2019
Point of Contact Priorie. (603) 570-0515	<ul> <li>TS8</li> <li>ORNL continued work on an initial prototype of a new NCSP Program Management Tool.</li> <li>The NCSP IER database on G2 required some updating in Q1 and access requests were approved as necessary.</li> <li>Worked with G2 programmers on required and desired IER database capabilities. This required multiple WebEx meetings to show the G2 programmers how the current database works and is used.</li> <li>A team of programmers are now working on this task to complete a prototype by sometime late Q2 or early Q3 for testing.</li> <li>TS11</li> <li>Worked to complete and publish the FY2019 integral experiment 5-year plan.</li> <li>ORNL conducted monthly integral experiment telecons and conducted a face-to-face meeting at Sandia in October. The C<sub>E</sub>DT manager tracked IER products and Baseline Change Reviews and worked with the NCSP manager to approve tasks, as required.</li> <li>Thomas Miller, C<sub>E</sub>DT Manager, resigned from ORNL in FY18Q4. Transition of C<sub>E</sub>DT duties back to Doug Bowen was initiated. A new CedT manager has been identified and will be announced in Q2. The new CedT manager has been identified and will be announced in Q2. The new CedT manager will begin work in Q3.</li> <li>All NCSP funded IERs were initiated in the IER database. Those experiments not funded were moved to a pending status.</li> <li>Bowen continued efforts to work with Tim Wynn (ORNL) and Ty Deschamp (NA-50) on the new IER database in G2. These meetings are frequent and on-going.</li> </ul>

### **ORNL TS Milestones:**

Complete	On Schedule	Behind Schedule	Missed Milestone

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Manage C <sub>E</sub> dT process and coordinate execution of planned IERs each FY. (TS2)		
	Maintain up-to-date spreadsheet of proposed tasks for NCSP Manager after the NCSP proposal review meeting and through the final task prioritization effort by the NCSP Management Team. (TS2)		
	Provide the NCSP manager with a summary of NCSP IE task TS11 as described in the task description. (TS11)		
Q2	Manage $C_E$ dT process and coordinate execution of planned IERs each FY. (TS2)		
	Maintain up-to-date spreadsheet of proposed tasks for NCSP Manager after the NCSP proposal review meeting and through the final task prioritization effort by the NCSP Management Team. (TS2)		
	Provide the NCSP manager with a summary of NCSP IE task TS11 as described in the task description. (TS11)		
Q3	Manage $C_E dT$ process and coordinate execution of planned IERs each FY. (TS2)		
	Maintain up-to-date spreadsheet of proposed tasks for NCSP Manager after the NCSP proposal review meeting and through the final task prioritization effort by the NCSP Management Team. (TS2)		
	Provide the NCSP manager with a summary of NCSP IE task TS11 as described in the task description. (TS11)		
Q4	Manage C <sub>E</sub> dT process and coordinate execution of planned IERs each FY. (TS2)		

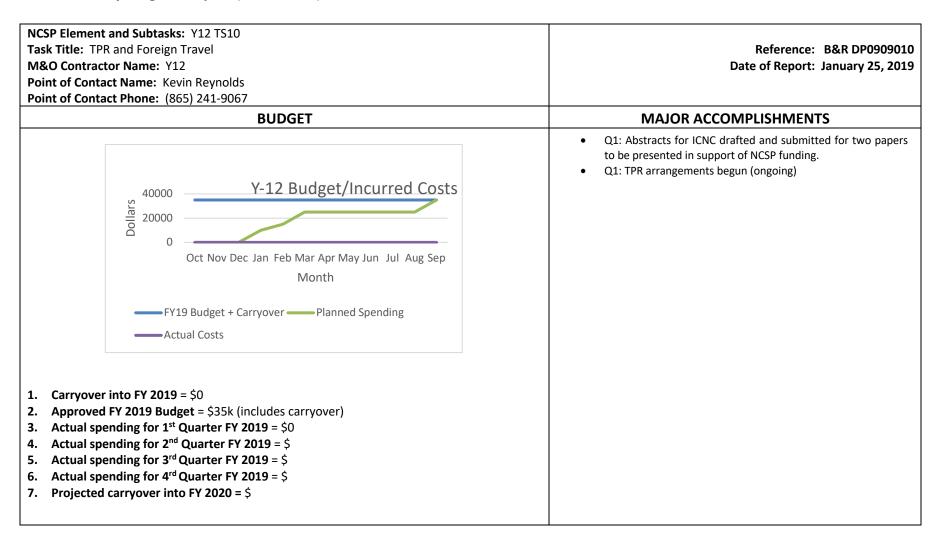
Ma	aintain up-to-date spreadsheet of proposed tasks for NCSP anager after the NCSP proposal review meeting and through the all task prioritization effort by the NCSP Management Team.
	described in the task description. (TS11)
	rticipate in Q4 Budget Execution Meeting and assist NCSP anager in finalization of approved tasks for next FY. (TS2)
Pub	blish final Five-Year Plan. (TS2)
	ovide NCSP Manager annual report of succession planning forts. (TS7)
	ovide NCSP Manager a status report of progress on the velopment of a program management tool. (TS8)



### SNL TS3 Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone	

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	NONE		
Q2	NONE		
Q3	NONE		
Q4	Provide NCSP Manager annual report of succession planning efforts.		



### Y12 TS10 Milestones:

Complete	On Schedule	Behind Schedule	Missed Milestone	

QUARTER	MILESTONE	STATUS	ISSUES/PATH FORWARD
Q1	Provide status reports all TPR hosting activities in NCSP Quarterly Progress Reports. (TS10)		
Q2	Provide status reports all TPR hosting activities in NCSP Quarterly Progress Reports. (TS10)		
Q3	Provide status reports all TPR hosting activities in NCSP Quarterly Progress Reports. (TS10) – only if still applicable		
Q4	Provide status reports all TPR hosting activities in NCSP Quarterly Progress Reports. (TS10) – only if still applicable		
	Provide Foreign Trip Report for ICNC. (TS10)		

# **STATUS REPORT**

### on the

# International Collaboration with the Atomic Weapons Establishment (AWE)

Reference			AWE Contributions and POCs				
AWE Reference	Task Description	NCSP Reference	FY2018 AWE Contribution	AWE Technical POC	Collaborator POC	DOE Lab	
Analytical Methods							
AWE-AM1	Slide rule update	ORNL-AM6 LLNL-AM3 IRSN-AM5	Perform calculations; attend meetings; review analysis and reports	R. JONES	M. DULUC	ORNL	
Performed calculation	s with Attila deterministic rad	liation transport code	e and fed into project lead. Reviewed p	ublications. AWE effort curren	itly on hold due to lack of reso	ource.	
INTEGRAL EXPERIMEN	NTS						
AWE-IE1	Inaugural international intercomparison of nuclear accident dosimetry using Flattop	LLNL-IE1 IRSN-IE15	Co-author final report (CED-4b)	C. WILSON	D. HICKMAN	LLNL	
CED-4b complete. The	ere is interest among participa	nts for publication in	a peer-reviewed journal and collabora	ition on unifying designs.			
AWE-IE2	Development of Passive Neutron Spectrometer (PNS)		Fully commission TLD version of the PNS; Perform validation irradiations at NPL; develop unfolding tools for directionality	C. WILSON	D. HICKMAN	LLNL	
			er on 4 <sup>th</sup> Feb to discuss fabrication. Test t detailing the design and testing of the			ntaneous fission	
AWE-IE3 IER 406	Cf-252 CAAS benchmark	LLNL-IE1 IRSN-IE28	Perform/support PNS(TLD) measurements with a shadow cone	C. WILSON	D. HEINRICHS	LLNL	
section of the ICSBEP			d into a single AWE Report and shared cated on LLNL fabrication of the cone,				
AWE-IE4 IER 175	Godiva-IV CAAS benchmark	ORNL-IE4 IRSN-IE27	Review of experiment design. Provide measurement capability as required	C. WILSON	T. MILLER	ORNL	
AWE has the reviewed	d the proposal.						
AWE-IE5	Correction factor for dosimetry linked to orientation of the victim	LLNL-IE1 IRSN-IE29	Participate in experiment design; use PNS data to determine directional components of neutron fields (Godiva, Flattop, LLNL RCL)	C. WILSON	D. HEINRICHS	LLNL	
AWE has compiled PN	S measurement data from Go	diva-IV, Flattop and I	LNL RCL. The development of a metho	od to unfold directional data ha	as not started.		
AWE-IE6	ICSBEP shielding benchmark for shipping containers	LLNL-IE13 IRSN-IE36	Participate in experiment design; PNS(TLD) could be deployed as primary measurement device	C. WILSON	S. KIM	LLNL	

Reference			AWE Contributions and POCs				
AWE Reference	Task Description	NCSP Reference	FY2018 AWE Contribution	AWE Technical POC	Collaborator POC	DOE Lab	
			AWE to do some preliminary design				
Not started.						·	
AWE-IE7 IER 153	Measure fission neutron spectrum shape using threshold activation detectors	LANL-IE3	Provide input into foil selection; use AWE unfolding codes to provide independent analysis. TBC AWE to provide foil suggestions per MYERS	C. WILSON	T. CUTLER B. MYERS	LANL	
AWE has had corresp	ondence with LANL and has of	fered to perform an	independent analysis of the measurem	ent data. Currently waiting fo	or data.		
AWE-IE8	Diagnostic development for measurement of correlated leakage radiations	LLNL-IE1	A feasibility study is being developed at AWE to ascertain suitable counting scenarios and methods. An experimental design will then be produced in the following years based upon the outcomes of this study	N. KELSALL	D. HEINRICHS	LLNL	
Liquid scintillation sys	stem has been developed for f	ast neutron counting	and will be tested in an experiment at	NCERC in Q3.			
AWE-IE9	(Neutron multiplicity experiments) AWE/LLNL NCT 5 year measurement campaign	LLNL-PROPOSAL 18	Participate in experiment design, measurements and reporting	N. KELSALL	D. HEINRICHS	LLNL	
AWE is producing a re	eport summarizing the measu	ements analyzed to	date. Aim to provide a presentation at	the Technical Program Reviev	v.		
AWE-IE10	Enhanced methods of criticality accident dosimetry No funding for FY19 awe will provide proposal for FY20	LLNL-IE1 IRSN-30 IRSN-33 Naval Dosimetry Center	Develop prototypes, participate in design, execution and reporting of dosimetry experiments	C. WILSON	F. TROMPIER	LLNL	
AWE is conducting so	me initial studies into new me	thods.					
AWE-IE11	International intercomparison of nuclear accident dosimetry AWE to assist in preliminary design FY19 and FY20	LLNL-IE18 SNL-IE4	Produce experiment design; participate in exercise; produce final report. Repeat 2 - 3 years	C. WILSON	D. HICKMAN	LLNL	
Have agreed in corres	spondence with IRSN and LLNI	that we should plan	for the next IC in 2021 (funding permit	tting). Design work not starte	d.		
AWE-IE12	CIDAAS testing	Proposal 20	Deploy AWE CIDAAS for test irradiation. Repeat 2 - 3 years	T. BIRKETT	J. SCORBY	LLNL	
AWE successfully test	ed CIDAAS in May 2018 and p	rovided support to C	ED-4.				

Reference			AWE Contributions and POCs				
AWE Reference	Task Description	NCSP Reference	FY2018 AWE Contribution	AWE Technical POC	Collaborator POC	DOE Lab	
AWE-IE13	Characterization of AFRRI TRIGA reactor radiation field AWE will provide onsite measurement	LLNL-IE18 SNL-IE4	Provide support to experiment design	C. WILSON	A. ROMANYUKHA	LLNL	
AWE has drafted the June 2018.	final design (CED-2) and distrib	outed to participants	for comment. AWE has coordinated th	e selection of a date for the ex	periment, set to the week co	mmencing 10 <sup>th</sup>	
INFORMATION PRESI	ERVATION AND DISSEMINATION	ON					
AWE-IPD1	Conduct benchmark evaluations of legacy IEU integral experiments Requires no NCSP funding	LLNL-IPD1	Assess feasibility of sponsoring PhD; determine availability of data	C. WILSON	D. HEINRICHS	LLNL	
Not started.							
TRAINING AND EDUC	ATION						
AWE-TE1	Hands-on criticality safety training	ORNL-TE1 LANL-TE1 LLNL-TE1 LLNL-TE3 SNL-TE1 IRSN-TE1	AWE personnel to attend training course	R. JONES	D. BOWEN B. MYERS D. HEINRICHS G. HARMS S. EVO (IRSN)	ORNL	
No current plans to a	ttend courses.						

### **STATUS REPORT**

### on the

# International Collaboration with the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) for FY2019

	REFERENCE		IRSN Contributio	n / POC		
IRSN Reference	Task Title	DOE Reference	FY 2019 IRSN Contribution	IRSN Technical POC	DOE Technical POC	DOE LAB
			Analytical Methods			
IRSN-AM15	MCNP Maintenance and Support / Uncertainty Analysis Development / Modernization / etc.	LANL-AM1	Interest for uncertainty analysis, source convergence development and modernization strategy	E. DUMONTEIL	F. BROWN	LANL
Forrest Brown'	s prescription (given in the frame of the I	MC subgroup at	OECD) to diagnose spatial correlations are being implemented	into MORET.		
IRSN-AM16	Multi-Physics Methods for Simulation of Criticality Excursions	LLNL-AM2	Technical exchanges on the proposed multiphysics tasks for simulating criticality excursions.	M. DULUC	D. HEINRICHS	LLNL
Task not starte	d.					
IRSN-AM1	Validation and qualification methods	ORNL-AM2 ORNL-IPD4	Covariance matrices establishment of the selection of Integral Experiments	I. DUHAMEL	D. BOWEN B. REARDEN	ORNL
	nitiated in the frame of the OECD/NEA UA eriments of interest for the FY2019.	ACSA expert grou	ip. Experimental correlations were established for LCT007 and	LCT039 – need to co	ntact Brad Rearde	n to discuss
IRSN-AM3	Monte Carlo & sensitivity calculations	ORNL-AM2	Technical exchanges on sources convergence issues, sensitivity coefficients calculations and kinetics parameters calculations	B. DECHENAUX	D. BOWEN B. REARDEN	ORNL
			ivity coefficients. Following this work, 2 methods were implem			
comparisons b	etween MORET and SCALE were done. The	ne kinetics param	neters calculation is already implemented in MORET 5. Nothing	g undertaken in FY201		
IRSN-AM5	Update of the slide rule	ORNL-AM6 LLNL-AM3 AWE-AM1	Subtask 2 of IRSN proposal Update of the "slide rule" for the rapid response estimation of a criticality accident (using COG, MCNP, MAVRIC, ATTILA)	M. DULUC	D. BOWEN D. HEINRICHS C. WILSON	ORNL LLNL AWE
Report in progr	ress. The next step will be in particular th	e number of fissi				
IRSN-AM7	ACE QA testing and implementation	LANL-AM2	Implementation of the defined QA tests in ACEtk and integration in GAIA	L. LEAL	J. CONLIN	LANL
Report provide	ed by LANL to IRSN by Wim Haeck with de	tailed descriptio	ns.			
IRSN-AM8	Analytical Methods Working Group	NCSP-TS2	IRSN participation to NCSP analytical methods Working Group and IRSN participation to TPR meeting	S. EVO	F. BROWN D. BOWEN	NCSP
Participation in	AMWG in March 2018. Next meeting in	March 2019.				
IRSN-AM9	Cross sections processing validation	ORNL-AM3	Development of an interface between GAIA and AMPX and test interface capabilities. AMPX training desired by IRSN staff in FY2019.	R. ICHOU	D. WIARDA D. BOWEN	ORNL
Tool for genera	ating AMPX multigroup cross section libra	ry with DRAGON	I. Task needs completion.			

	REFERENCE		IRSN Contribution / POC					
IRSN Reference	Task Title	DOE Reference	FY 2019 IRSN Contribution	IRSN Technical POC	DOE Technical POC	DOE LAB		
IRSN-AM13	Benchmark intercomparison study	LLNL-AM5 ORNL-AM10 LANL-AM5	Definition of common set of developed benchmark models Calculations for Pu and HEU systems. (Completion of this task before ORNL-AM9 and LANL-AM4 would be useful to identify common benchmarks.)	I. DUHAMEL	D. HEINRICHS D. BOWEN F. BROWN	LLNL ORNL LANL		
IRSN-AM13 in	progress –Results from different labs coll-	ected – prelimin	ary analyses done $ extcolor{black}{ o}$ feedback on COG and MORET input deck	s – common paper for	ICNC (abstract s	ubmitted)		
IRSN-AM14	Sensitivity/Uncertainty comparison study with a focus on Upper Subcritical Limits	ORNL-AM9 LANL-AM4	Definition of three test cases Calculations and intercomparison technical report	I. DUHAMEL	F. BROWN D. BOWEN	LANL ORNL		
In progress – I		results with MA	CSENS are being analysed $ ightarrow$ some issues with MACSENS dev.					
IRSN-AM17	Technical Data for the Pitzer Formulation of Solution Compositions to Include Uranium/Plutonium Solutions with Selected Admixed Absorbers	ORNL-AM16 LANL-AM6 LLNL-AM7	Contribution to measurements definition. Comparison of density laws (isopiestic law for instance)	N. LECLAIRE	D. BOWEN	ORNL		
issues, the act	·	tonium sulfate o		-	-			
			Integral Experiments					
IRSN-IE1 <b>IER 184</b>	TEX - Ta experiment	LLNL-IE4	Sensitivity/uncertainty calculations Contribution to the evaluation of the first experiments.	M. BROVCHENKO	C. PERCHER	LLNL		
2015, IRSN pe	rformed sensitivities calculations on the d	esigned configu	nated in the kick-off meeting. IRSN is part of the CED team and rations for TEX-Ta experiments. Regular VTC were organized to e ICSBEP evaluation in 2019 as independent reviewer.					
IRSN-IE3 IER 209	New 7uPCX experiment	SNL-IE1	Contribution to ICSBEP reevaluation.	N. LECLAIRE	G. HARMS	SNL		
These experim	nents were finally not presented at the Oc	tober 2018 mee	ting					
IRSN-IE6 IER 306	Rh foils experiment	SNL-IE1	IRSN proposal: preliminary evaluation of experimental uncertainties prior to the experiment's CED-2 report.	N. LECLAIRE	G. HARMS	SNL		
	s in the IRSN validation process and will be n 2019. (supported by a sub-contract)	e issued in Marc	h 2019. Preliminary effects on keff of experimental uncertainti	es have been calculate	ed and will be ad	ded in the		
IRSN-IE7 IER 305	Mo foils and rods experiment	SNL-IE1	IRSN proposal: Leading the CED-3a report; Supplying the Mo rods for the experiment.	N. LECLAIRE	G. HARMS	SNL		
	·	•	ld not be totally done in 2019. We looked at potential supplier	rs for the Mo sleeves a	and estimated the	e costs.		
	waited for the CED-2 report to be finished T	before proceed						
IRSN-IE8 <b>IER 451</b>	Ti experiment	SNL-IE1	Analysis of the experiments Comparison with MIRTE program	N. LECLAIRE	G. HARMS	SNL		
			er 2018 meeting. The experiments were calculated with MORE			611		

subcontract in 2019.

	REFERENCE		IRSN Contribution	on / POC		
IRSN Reference	Task Title	DOE Reference	FY 2019 IRSN Contribution	IRSN Technical POC	DOE Technical POC	DOE LAB
IRSN-IE11 IER 297	TEX - Hf experiment	LLNL-IE4	Contribution to Jemima plates characterization. Contribution to CED report.	M. BROVCHENKO	C. PERCHER	LLNL
	ved in the review of the CED2 report and d-by, waiting from LLNL	provide some se	ensitivity calculations to LLNL. The status of the program has b	een discussed regularl	y during VTC unti	il 2017 with
IRSN-IE15 IER 253	International intercomparison exercise using FLATTOP	LLNL-IE1 AWE-IE3	Participation in the design, contribution to the experiments with IRSN materials, and the report.	M. DULUC F. TROMPIER	D. HEINRICHS C. WILSON	LLNL AWE
Exercise done	in May 2018. Report in progress.					
IRSN-IE19	Solution reactor	Y12-IE2	Strong IRSN interest for participation in the design, specification of a solution reactor	M. DULUC	P. ANGELO	Y-12
Task started. A	A first contact with Peter.					
IRSN-IE25 IER 296	TEX - MOX experiment	LLNL-IE4	IRSN leads this proposal for design and will author the CED-1 & 2 reports with LLNL support. Characterization of moderator and reflector plates. IRSN contribution to the moderator and reflector plates funding.	M. BROVCHENKO	C. PERCHER	LLNL
Design optimiz	zation for TEX-MOX ongoing. (Supported b	y sub-contracts	in 2018 and 2019)	1		
IRSN-IE26 IER 295	TEX - Iron experiment	LLNL-IE4	Contribution to the experiments design. Contribution to CED reports and review.	M. BROVCHENKO	C. PERCHER	LLNL
This task is on	stand-by for NCSP					
IRSN-IE27 IER 175	GODIVA CAAS benchmark	ORNL-IE4	Participation in the design. Provide IRSN materials for irradiation, analysis of results.	M. DULUC	T. MILLER	ORNL
Task not starte	ed.					
IRSN-IE28 IER 406	Cf-252 CAAS benchmark	LLNL-IE1	Participation in the design. Provide IRSN materials for irradiation, analysis of results	M. DULUC F. TROMPIER	D. HEINRICHS	LLNL
Discussion in p	progress to perform additional measurement	ent in 2019.				
IRSN-IE29	Correction factor for dosimetry linked to the orientation of the victim	LLNL-IE1 AWE-IE7	Participation in the design. Provide IRSN materials for irradiation, analysis of results.	M. DULUC F. TROMPIER	D. HEINRICHS C. WILSON	LLNL AWE
Task not starte						
IRSN-IE30	Full dosimetry exercise around GODIVA/FLATTOP reactors	LLNL-IE1	Participation in the design. Provide IRSN materials for irradiation, analysis of results	M. DULUC F. TROMPIER	D. HEINRICHS	LLNL
Task not starte	ed					
IRSN-IE33	Sodium activation experiment around GODIVA/FLATTOP	LLNL-IE1	Participation in the design. Provide IRSN materials for irradiation, analysis of results	M. DULUC F. TROMPIER	D. HEINRICHS	LLNL
Task not starte	ed					
IRSN-IE34	HEU critical and Subcritical measurements	LANL-IE23	Participation in the definition and the design of the experiment	W. MONANGE	J. HUTCHINSON	LANL
Task not starte	ed					
IRSN-IE35 IER 434	Godiva benchmark for time dependent code validation	LANL-IE3	Participation in the preliminary design and CED-1 report.	M. DULUC	J. GODA	LANL

	REFERENCE		IRSN Contribution / POC				
IRSN Reference	Task Title	DOE Reference	FY 2019 IRSN Contribution	IRSN Technical POC	DOE Technical POC	DOE LAB	
Task not starte	ed						
IRSN-IE36	ICSBEP Shielding benchmarks for shipping containers	LLNL-IE13 AWE-IE8	Participation in the preliminary design and CED-1 report	M. DULUC	D. HEINRICHS C. WILSON	LLNL AWE	
Task not starte	ed						
IRSN-IE37	Critical and subcritical measurements with a Zero-Power research reactor (On going task)	LANL-IE21	Analysis of the experiments, participation in the final technical report.	E. DUMONTEIL	J. HUTCHINSON	LANL	
Design studies	in 2016 and 2017. The experiment occur	red in 2017. The	final simulations were completed end of 2018 and the analysi	s is in progress.			
IRSN-IE39	Thermal/Epithermal Experiments (TEX) Plutonium Experiments at Low Temperatures	LLNL-IE19	Participation in experiments design and CED reports. To be discussed with LLNL.	M. BROVCHENKO	D. HEINRICHS	LLNL	
Task not starte	ed.						
IRSN-IE40	CAAS performance testing	LLNL-IE21	Participation in testing activities. Provide IRSN materials and French CAAS probes. To be discussed with LLNL.	M. DULUC	D. HEINRICHS	LLNL	
Task not starte	ed						
IRSN-IE41	Thermal/Epithermal Experiments (TEX) with Chlorine and Lithium	LLNL-IE23	Participation in experiments design and CED reports. To be discussed with LLNL.	M. BROVCHENKO	D. HEINRICHS	LLNL	
Task not starte	ed.			l			
		Inf	ormation Preservation and Dissemination				
IRSN-IPD1	ICSBEP reviewing	LLNL-IPD1	IRSN ICSBEP reviewing tasks are reported in the IE tasks	I. DUHAMEL	D. HEINRICHS	LLNL	
ICSBEP reviews	s of SCRAP, ISSA and titanium experiment	s in October 201	8 – Review of TEX-Ta planned for the Q4 of FY 2019 (if evaluat	tion is proposed)			
IRSN-IPD3	ICSBEP benchmark reviewing	LLNL-IPD1	IRSN ICSBEP reviewing tasks	I. DUHAMEL	J. FAVORITE	LANL	
Not started – v	waiting for FLATTOP reevaluation						
			Nuclear Data				
IRSN-ND1	Contribution to new evaluations	ORNL-ND1	Contribution to new evaluation and validation for <sup>54</sup> Fe, <sup>103</sup> Rh, <sup>55</sup> Mn and Gd isotopes	L. LEAL	D. BOWEN	ORNL	
	•		preliminary resonance evaluation generated. IRSN benchmark Improved Gd resonance parameters available.	assembled for testing	g the 55Mn evalua	tion. New	
IRSN-ND2	Nuclear data processing	LANL-ND1	Benchmark testing of <sup>235</sup> U and <sup>239</sup> Pu cross section library	L. LEAL	J. CONLIN	LANL	

	REFERENCE		IRSN Contribution / POC								
IRSN Reference	Task Title	DOE Reference	FY 2019 IRSN Contribution	IRSN Technical POC	DOE Technical POC	DOE LAB					
Test performed and new <sup>235</sup> U and <sup>239</sup> Pu resonance parameters generated.											
IRSN-ND3	Nuclear data processing	LLNL-ND4	Resonance evaluation of <sup>233</sup> U (Pending prioritization of <sup>233</sup> U ND tasks for the NCSP)	L. LEAL	D. HEINRICHS	LLNL					
Existing resonance evaluation extended to 2 keV. New resonance parameters derived.											
Training and Education											
IRSN-TE1	Hands-on criticality safety training	ORNL-TE1 LANL-TE3 LLNL-TE1 SNL-TE1	IRSN attendance to NCSP classes. Possible lectures by IRSN working with NCSP training and education coordinator.	S. EVO	D. BOWEN	NCSP					
2 IRSN staff at	tending the hands-on training in January 2	-	1	ı	1						